

4th International Turkish Congress on Molecular Spectroscopy
05-09 August 2019 Kusadasi, Aydin, Turkey

TURCMOS 2019



2019 AUGUST 05-09

Kusadasi | Turkey

ABSTRACT BOOK



K U S A D A S I T U R K E Y

AUGUST 05-09

2019

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WELCOME TO TURCMOS 2019,

On behalf of the Scientific and Organizing Committee, we would like to welcome you all to the **“4th International Turkish Congress on Molecular Spectroscopy (TURCMOS2019)”**. The scope of the congress is to encourage the exchange of ideas and future collaborations all around the world, introduce new techniques and instruments, and present recent developments in this field of research. In the congress, all aspects of spectroscopic methods as well as related computational and theoretical approaches will be considered. Contacts between young researchers (M.Sc. and Ph.D.) and prominent experts will be particularly stimulated, aiming at the development of future collaborations.

We would like to express our acknowledgments to official venue hotel, sponsors and Leon Congress for their support.

We hope that the congress will provide you intellectual and social experience. We wish you enjoyable week in Kusadasi.

Ozan UNSALAN

President

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**Alphabetically ordered by surname.*

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Scientific Program

DETAILED SCIENTIFIC PROGRAMME	
5 August 2019, Monday	
09.15 – 09.30	Opening Ceremony
Chair: Ozan UNSALAN	
09.30 – 10.20	PL1 – Juergen POPP <i>Clinical Raman Spectroscopy – Precise Diagnosis as the basis for Individual and Targeted Therapy</i>
10.20 – 11.10	PL2 – Sefik SUZER <i>X-Ray Photoelectron Spectroscopy, a Chemical Tool for Electrochemical Analyses of Potential Developments at Liquid/Solid Interfaces: Past, Present and Future</i>
11.10 – 11.30	Coffee Break
11.30 – 11.50	O1 – Marco PINTO CORUJO <i>Characterization of Proteins by Vibrational Spectroscopy</i>
12.00 – 13.30	Lunch Break
Chair: Marco PINTO CORUJO	
14.00 – 14.20	O2 – Mustafa UNAL <i>Development of a Spatially Offset Raman Spectroscopy Method for non-invasive Assessment of Bone Quality</i>
14.20 – 14.40	O3- Shadi SADIGH <i>Investigation of the Effect of α-Lipoic Acid on Liver Cell Damage in Acitretin and Methotrexate Given Rats</i>
14.40 – 15.00	O4 – Gamze TAN <i>Biosynthesis and Characterization of Gold Nanoparticles using Persea Americana Leaf Extract</i>
15.00 – 15.20	Coffee Break
Chair: Mustafa UNAL	
15.20 – 15.40	O5 – Ozlem BOZKURT-GIRIT <i>Diabetes Induces Structural Alterations in Proteins and Lipids in Kidney Glomeruli</i>
15.40 – 16.00	O6 – Dursun KARAAGAC <i>Synthesis, Spectroscopic, Thermal, and Structural Properties of Three New Bimetallic Cyano-Bridged Coordination Polymers Containing 4-aminomethylpyridine</i>
16.20 – 16.40	O7– Hilal ACAY <i>Green Synthesis, Characterization of Gold Nanoparticles Using the Aqueous Extract of Russula delica</i>
18.00 – 19.00	Welcome Party

DETAILED SCIENTIFIC PROGRAMME	
6 August 2019, Tuesday	
Chair: Weitao YANG	
09.30 – 10.20	PL3 – Resat APAK <i>Applied Molecular Spectroscopy in Optical Sensor Design for Antioxidant and Energetic Compounds</i>
10.20 – 11.10	PL4 – Austin NEVIN <i>Material History: Recent Research and New Insights into the Use of Binding Media, Meteoritic Iron and Red Lakes</i>
11.10 – 11.30	Coffee Break
11.30 – 11.50	O8 – Miroslav DRAMIĆANIN <i>Photoluminescence of Mn⁴⁺ Activated Li₂TiO₃: The Route for Highly-Sensitive Luminescence Thermometry</i>
12.00 – 13.30	Lunch Break
Chair: Miroslav DRAMIĆANIN	
14.00 – 14.20	O9 – Gunnur GULER <i>Discrimination of Cancer Cell Subpopulations based on FTIR Spectral Data</i>
14.20 – 14.40	O10- Mehmet BAY <i>Investigation of Large-Area MoSe₂ Monolayer Formation using NaCl Salt Catalyzer by Raman Scattering and Photoluminescence Spectroscopy</i>
14.40 – 15.00	O11 – Mustafa TUZEN <i>A New, Simple and Green Switchable Solvent Extraction of Rhodamine B and its Spectrophotometric Determination in Water, Food and Soft Drink Samples</i>
15.00 – 15.20	Coffee Break
Chair: Austin NEVIN	
15.20 – 15.40	O12 – Aytac LEVET <i>Neutron Measurements for Ferro Boron Alloys and Experimental Determination of Radiation Properties</i>
15.40 – 16.00	O13 – Ozan UNSALAN <i>Evidence of Maskelynite Formation and Low Weathering of Didim Meteorite by Infrared and EDXRF Spectroscopy</i>
16.00 – 18.00	Poster Session Poster No : 01 - 13

DETAILED SCIENTIFIC PROGRAMME	
7 August 2019, Wednesday	
Chair: Resat APAK	
09.30 – 10.20	PL5 – Weitao YANG <i>Fractional Perspectives and Quasiparticle and Excitation Energies from Ground State DFT Calculations</i>
10.20 – 11.10	PL6 – Tolou SHOKUHFAR <i>In-Situ TEM Studies of Biomineralization</i>
11.10 – 12.00	PL7 – Reza SHAHBAZIAN-YASSAR <i>Two-Dimensional Materials and 3D Printing of Li Batteries</i>
12.00 – 12.10	Coffee Break
Chair: Michael OSHTRAKH	
12.10 – 12.30	O14 – Duygu BARUT CELEPCI <i>Theoretical Studies and Spectroscopic FT-IR and NMR Comparisons of Two Pd-based N-heterocyclic carbene Complexes</i>
12.30 – 12.50	O15 – Lamia AÏSSAOUI <i>Open Shell Ions Mobility in Cooled Helium Gas at 4.3K: Shallow Minimum Appearance</i>
12.50 – 13.10	O16- Med Taieb BEN DHIA <i>DFT and-[¹H, ³¹P, ¹¹⁹Sn]-NMR Investigation of the Cis-Trans Isomerization Mechanism of the Adduct SnCl₄.2HMPA* Complex</i>
13.10 – 14.00	Lunch Break
14.00 – 19.00	Social Tour

DETAILED SCIENTIFIC PROGRAMME	
8 August 2019, Thursday	
Chair: Angelina POPOVSKA	
09.30 – 10.20	PL8 – Thomas MAVROMOUSTAKOS <i>Drug Delivery Systems for Optimizing the Therapeutic Index</i>
10.20 – 10.40	O17 – Yuliya E. TYUTEREVA <i>Short-Lived Intermediates in Photochemistry of p-Arsanilic Acid: A Laser Flash Photolysis Study</i>
10.40 – 11.00	Coffee Break
Chair: Med Taieb BEN DHIA	
11.00 – 11.20	O18 – Ahmet EMIR <i>Phenolic Profiling of Allium scorodoprasum subsp. rotundum by LC-MS/MS and Evaluation of Its Biological Activity</i>
11.20 – 11.40	O19 – Oguz CAKIR <i>Studies of Imprinting Conditions and Recognition Performance of Pirimicarb-Imprinted Sensor Chip</i>
11.40 – 12.00	O20 – Hamdi TEKIN <i>A Review of Studies on Monitoring of Self-Healing Processes by the help of Different Types of Spectroscopy</i>
12.00 – 13.30	Lunch Break
Chair: Cisem ALTUNAYAR-UNSANLAN	
13.40 – 14.40	Sponsor Presentation (SEM) Evren ERDEM <i>The Agilent Cary 3500 UV-Vis Spectrophotometer Offers Photometric Performance together with Unique Measurement Capabilities</i> Berk MUJDE <i>Agilent Cary 7000 Universal Measurement Spectrophotometer</i>
14.40 – 15.00	Coffee Break
15.00 – 16.00	Workshop on NMR Thomas MAVROMOUSTAKOS <i>Structure Elucidation of Active Materials Using 1D and 2D NMR Spectroscopy</i>
16.00 – 18.00	Poster Session Poster No : 14 – 25
19.00 – 00.00	Gala Dinner

DETAILED SCIENTIFIC PROGRAMME	
9 August 2019, Friday	
Chair: Thomas MAVROMOUSTAKOS	
09.30 – 10.20	PL9 – Michael OSHTRAKH <i>Nondifferentiated and Differentiated Stony Meteorites: Comparative Analysis Using X-Ray Diffraction, Magnetization Measurements and Mössbauer Spectroscopy</i>
10.20 – 10.40	Coffee Break
10.40 – 11.00	O21 – Cigdem DONMEZ GUNGUNES <i>Investigation of the Properties of a Magnetically Modified Chestnut Shell Nanobiosorbent using Mössbauer Spectroscopy and FTIR</i>
11.00 – 11.20	O22 – Cisem ALTUNAYAR-UNSANAN <i>A Biophysical Study of the Interactions between Citrus Flavonoid Hesperidin and Membrane Lipids</i>
11.20 – 11.40	Closing Ceremony
12.00 – 13.30	Lunch Break
LEAVING THE VENUE	

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Poster List

POSTER SESSION 1 (P-01 / P-13) | August 06, 2019 - Tuesday

Number	Abstract title Authors
P-01	New 5-arylidene-4-thiazolidinone, Synthesis, UV/Vis-Absorption and Fluorescence Spectroscopic Rosa Nechak, <u>Samia Bouzroua-Achouche</u> , Sophie Poulain-Martini and Elisabet Duñach
P-02	An Efficient and Catalytic One-Pot Coupling Method for the Synthesis of Novel Pyran and Furan Derivatives Naouel Boufroua, <u>Samia Bouzroua-Achouche</u> , Sophie Poulain-Martini and Elisabet Duñach
P-03	Spectroscopic Identification of Pigments Used in Icons from the Church St. George, Struga Svetlana Mamucevska-Miljkovikj, <u>Angelina Popovska</u> , Zita Szikszai, Zsófia Kertész, Živko Kokolanski and Matthew Gri
P-04	The Role of the Nanoparticles Systems with Vitamins B on the Stratum Corneum <u>Adéla Jenišťová</u> , Ondřej Stuchlík, Vadym Prokopec and Pavel Matějka
P-05	Label-Free Bacteria Detection and Discrimination Using Raman and Ultrasensitive Surface-Enhanced Raman Spectroscopy <u>Alia Colniță</u> , Nicoleta Elena Dina, Nicolae Leopold, Dan Cristian Vodnar, Diana Bogdan, Sebastian Alin Porav and Leontin David
P-06	Polymethylsilsequioxane Concentration Effects on the Nanostructures and the Biophysical Properties of Some Foundations and BB Creams <u>Pinar Kaya</u> , Damla Karaarslan, Chun-Jen Su, Akin Bacioglu, Sinem Diken Gur, Sevgi Bayari, U-Ser Jeng and Semra Ide
P-07	Contribution of Infrared Spectrophotometry in the Analysis of Urolithiasis <u>Abdelatif Boutefnouchet</u> , Asma Lekouaghet, Khaoula Ghenaiet and Rim Mecheri
P-08	2D Structures in Full-Biobased Polyamide Nanocomposites Characterized by Raman Spectroscopy <u>Ioana Brezestean</u> , Daniel Marconi, Alia Colniță, Roxana Pasca, Andreea Alexandra Măineia, Nicoleta Levintă and Ioan Turcu
P-09	Influence on the Experimental Conditions on the SERS Signal of Nodularin Cyanotoxin <u>Ioana A. Brezestean</u> , Fran Nekvapil, Müller Molnár Csilla, Leontin David, Vasile Chis and Simona Cinta Pinzaru
P-10	The Effect of Methotrexate on Testis Sevil Iplikcioglu, Emine Diraman, Fatma Gonul Solmaz and <u>Shadi Sadigh</u>
P-11	Characterisation of Produced Lipid from a Green Microalgae <u>Zulfiye Velioglu Tosuner</u> and Raziye Ozturk Urek
P-12	DFT Study of Band Structure of Poly(telluro[3,4b]tellurophene) <u>Zeki Buyukmumcu</u>
P-13	The Use of Raman Spectroscopy in Forensic Sciences <u>Aylin Yalcin Saribey</u>

POSTER SESSION 2 (P-14 / P-25) | August 08, 2019 - Thursday

Number	Abstract title Authors
P-14	DFT Study of Polytellurophene as a H ₂ O Sensor <u>Fatma Selampinar</u> and Zeki Buyukmumcu
P-15	The Theoretical Investigation of Structural, Spectroscopic and Thermodynamic Properties of Palmitoleic Acid <u>Tugba Gocen</u> and M. Haluk Guven
P-16	Spectroscopic and Thermal Study of 3D-Metal Complexes with Pyrazolecarboxylic Acid Grzegorz Świdorski, Karolina H. Markiewicz, Monika Kalinowska, Renata Świśtocka, Marzena Matejczyk and <u>Włodzimierz Lewandowski</u>
P-17	Spectroscopic Study on Alkali Metal Salts of Rosmarinic Acid <u>Renata Świśtocka</u> , Ewa Regulska, Joanna Karpińska, Grzegorz Świdorski, Marzena Matejczyk, Aleksandra Golonko and <u>Włodzimierz Lewandowski</u>
P-18	Pro-, Antioxidant, Cytotoxic (toward MCF-7 and MDA-MB-21 Cell Lines), Lipophilic and Antimicrobial Activity of Hydroxybenzoic Acids <u>Monika Kalinowska</u> , Sylwia Męczyńska-Wielgosz, Anna Pietryczuk, Adam Cudowski, Barbara Złowodzka, Renata Świśtocka, Grzegorz Świdorski and <u>Włodzimierz Lewandowski</u>
P-19	Comparision of Spectroscopic and Thermal Properties of 3D-Metal Complexes with Nicotinic and Quinolinic Acid <u>Grzegorz Świdorski</u> , Agnieszka Z. Wilczewska, Renata Świśtocka, Monika Kalinowska and <u>Włodzimierz Lewandowski</u>
P-20	The Effects of the Metallic Synergy in the Barbiturate and Borat Complexes on Thermal Degradation of PVC Ilkan Kavlak, <u>Seray Kekec</u> and Gunes Suheyyla Kurkcuoglu
P-21	The Investigation of Thermal Stabilization Properties of the M(II) Barbiturate Complexes in the PVC Mold Ilkan Kavlak, <u>Seray Kekec</u> and <u>Güneş Suheyyla Kurkcuoglu</u>
P-22	Strong Shock Indication in Kemer Meteorite: Implications from Infrared Spectroscopy <u>Ozan Unsalan</u> and Cisem Altunayar-Unsalan
P-23	Donor-Acceptor π -conjugated Naphtalene Bis-benzimidazole: A DFT, Infrared and Raman Spectroscopic Study on a Heterojunction Solar Cell <u>Ozan Unsalan</u> , Cisem Altunayar-Unsalan, Yusuf Sert and <u>Sule Erten-Ela</u>
P-24	Vibrational Spectroscopic and DFT Investigation on Electron Acceptor Perylene Bisbenzimidazole <u>Ozan Unsalan</u> , Cisem Altunayar-Unsalan, Yusuf Sert and <u>Sule Erten-Ela</u>
P-25	Characterization of Proteins by Vibrational Spectroscopy and Self-Organizing Maps <u>Marco Pinto Corujo</u> , Maurizio Muroli, Nikola Chmel, Lindo Vivian and Alison Rodger

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Invited Speakers' Abstracts

PL-01

Clinical Raman Spectroscopy – Precise Diagnosis as the basis for Individual and Targeted Therapy

Jürgen Popp

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Understanding the causes of diseases, recognizing them earlier and treating them more specifically - hopes that are associated with modern biomedicine - requires the determination of diagnostic, prognostic and predictive factors including their comprehensive evaluation in just a few steps or ideally in a single step. In this context, the sharp rise in cancer due to an ageing society and the rapid spread of life-threatening infectious diseases (due in part to unknown pathogens) and antibiotic-resistant germs, which is partly due to increasing worldwide mobility but also to the ill-considered administration of broad spectrum antibiotics, should be mentioned in particular. An effective and early diagnosis and personalized therapy of cancer and infections requires new methods of differential diagnosis and represents an outstanding task of medicine. In principle, the following applies to all diseases: the earlier treatment begins, the better the chances of cure. There is therefore a great need for new diagnostic methods for targeted early diagnosis of diseases in order to be able to use targeted therapy as early as possible. Light plays a key role in the implementation of these ambitious goals. The use of optical technologies in medical diagnostics and therapy has increased rapidly over the last 10 years. Thereby photonic research is supported by advances in the field of digitization for the automated evaluation of optical data using methods of artificial intelligence, or for the online display of optical measurement signals via augmented/virtual reality. Here we present examples at the interface optics/photonics and digitization for personalized medical diagnostics and therapy. We will introduce a series of innovative multi-contrast marker free spectroscopy approaches for (I) rapid diagnosis of infectious diseases for targeted antibiotic administration, which is crucial for the survival of patients (e.g. in a sepsis); (II) precise intraoperative tumor margin control, because reliable tumor margin recognition during an intervention is the key to effective tumor treatment; and (III) early diagnosis of neurodegenerative diseases of the fundus of the eye.

Acknowledgements

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PL-02

X-Ray Photoelectron Spectroscopy, a Chemical Tool for Electrochemical Analyses of Potential Developments at Liquid/Solid Interfaces: Past, Present and Future

Sefik Suzer

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Charge distribution, storage and movement in solutions and soft-matter are of paramount importance for understanding and intelligent use of various electrochemical concepts towards advanced applications in energy, chemical, biochemical, microfluidics and sensing. Over the last three decades the vast research efforts using advanced measurement, computational and simulation techniques have changed the old concept of electroneutrality assumed, and most of the time enforced, to be obeyed in many physicochemical processes taking place in solution surfaces or in pores of solid materials. Being a chemically sensitive and quantitative surface analysis technique, x-ray photoelectron spectroscopy (XPS) has been the pivotal method to extract information about distribution of cations and anions on various surface structures, once difficulties in handling liquids had been overcome through multiple advancements in experimental techniques. The pioneering XPS investigation of ion enrichment on surfaces of viscous liquids by H. Siegbahn [1], was later successfully extended to aqueous solutions in the form of micro-droplets, using synchrotron based photoemission spectroscopy by Faubel and coworkers [2]. In parallel, developments in ambient pressure XPS have enabled investigation of a large variety of critical materials and chemical processes [3]. All of these giant leaps and developments have also been successfully supported and guided by extensive molecular dynamics simulations. Nonvolatile room temperature ionic liquid (RTIL) electrolytes have allowed us and others to utilize lab-based XPS instruments for investigating various electrochemical processes under ultrahigh vacuum conditions, without the need for extensive pumping techniques nor synchrotron facilities. In this contribution, we report on using a similar multi-layered graphene as the top electrode and utilize XPS to monitor in-situ; (i) the changes in the anion/cation intensity ratio under applied electric fields, and (ii) the electrical potential developments on different surface structures, which are derived from the shifts in the binding energies of the corresponding atomic core levels in a chemically resolved fashion [4-6].

Keywords: Vibration; Spectroscopy; Polymer fibres; Solid electrolytes; Nanoparticles.

[1] Siegbahn, H., J. Phys. Chem. 1985, 89, 897-909.

[2] Winter, B. Faubel, M., Chem. Rev. 2006, 106, 1176-1211.

[3] Bluhm, H., Andersson, K., Araki, T., Benzerara, K., Brown, G. E., Dynes, J. J., Ghosal, S., Gilles, M. K., Hansen, H.C., Hemminger, J., J. Electron Spectrosc. Relat. Phenom. 2006, 150, 86-104.

[4] Camci, M., Aydogan, P., Ulgut, B., Kocabas, C., Suzer, S., Phys. Chem. Chem. Phys. 2016, 18, 28434-28440.

[5] Camci, M. T., Ulgut, B., Kocabas, C., Suzer, S., ACS Omega 2017, 2, 478-486.

[6] Camci, M. T., Ulgut, B., Kocabas, C., Suzer, S., J. Phys. Chem. C 2018, DOI: 10.1021/acs/jpc.8b02759.

PL-03

Applied Molecular Spectroscopy in Optical Sensor Design for Antioxidants and Energetic Compounds

Resat Apak

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The CUPRAC (CUPric Ion Reducing Antioxidant Capacity) spectrophotometric assay, launched in 2004 by our research group, has served the scientific/technological community for the last 15 years in determining the total antioxidant capacity (TAC) or activity of food and biological antioxidants [1]. The CUPRAC chromophore, i.e. cupric-neocuproine chelate absorbing light at 450 nm, is formed at the end of the redox reaction with antioxidants. The sensitivity and selectivity of the CUPRAC assay arise from the metal-to-ligand charge-transfer interactions and favourable redox potential, respectively. CUPRAC has been transformed into an optical sensor format utilizing a Nafion membrane [2], and coupled to both online-HPLC and nanotechnological [3] methods. The inadequacies of other spectroscopic antioxidant capacity assays will also be discussed, in comparison to the CUPRAC assay. Optical sensors offer advantages such as low cost, flexibility, remote control, speed, miniaturization and on-site/in situ analysis. Nanotechnology has been incorporated into optical sensors to increase the rate of reactions and the sensitivity of analytical determinations. To cite some examples, our research group utilized the localized surface plasmon resonance (LSPR) absorption of silver nanoparticles to develop a linear-response antioxidant sensor via enlargement of citrate-reduced seed particles by antioxidant addition [4]. We selectively determined biothiol-type antioxidants with Ellman reagent-derivatized gold nanoparticles (AuNPs) [5]. We designed a sensitive colorimetric method for nitrite (a food preservative), based on its colorimetric determination using 4-aminothiophenol-modified AuNPs and naphthylethylene diamine as coupling agent for azo-dye formation [6]. Nitrite also arises from the hydrolysis of nitramine explosives, detectable by the same method.

In field/on site detection and determination of explosive residues require rapid colorimetric sensing applications that may replace the more sophisticated, but high-cost LC/GC-MS/MS techniques (especially in screening analysis of post-blast debris). In this respect, our energetic compounds detection group has developed various colorimetric kits, spectroscopic sensors and nanoprobcs utilizing the electron-transfer (ET) and charge-transfer (CT) ability of explosive compounds. Intra-molecular (e.g., Meisenheimer anions of TNT after the addition of hydroxide, alkoxide or acetate to the aromatic ring) or inter-molecular CT (e.g., between TNT and dicyclohexylamine) interactions were used to spectroscopically quantify nitro-aromatic explosives, which were also converted to optical sensors [7,8]. We also manufactured a field colorimetric kit to detect explosive residues in the field (retained on a chromatographic paper) as determined by their color change after successively spraying on

paper three reagents which were specific for nitro-aromatics, nitramines/nitrate esters, and inorganic nitrates [9]. We recently designed a practical AuNPs-based colorimetric sensor for the determination of nitroaromatic explosives (TNT and tetryl), capable of analyte detection at picomolar levels, by derivatizing thioglycolic acid (TGA)-modified AuNPs with counter-charged (\pm)-trans-1,2-diaminocyclohexane (DACH) at optimal pH [10].

- [1] R. Apak, K. Güçlü, M. Özyürek, S. E. Karademir, J. Agric. Food Chem. 52 (2004) 7970.
- [2] M. Bener, M. Özyurek, K. Güçlü, R. Apak, Anal. Chem. 82 (2010) 4252.
- [3] M. Bener, F. B. Şen, R. Apak, Talanta 187 (2018) 148.
- [4] M. Özyürek, N. Güngör, S. Baki, K. Güçlü, R. Apak, Anal. Chem. 84 (2012) 8052.
- [5] K. Güçlü, N. Güngör, M. Özyürek, S. Baki, R. Apak, Anal. Chim. Acta 794 (2013) 90.
- [6] A. Üzer, Z. Can, I. Akın, E. Erçağ, R. Apak, Anal. Chem. 86 (2014) 351.
- [7] A. Üzer, E. Erçağ, R. Apak, Anal. Chim. Acta 505 (2004) 83.
- [8] E. Erçağ, A. Üzer, R. Apak, Talanta 78 (2009) 772.
- [9] E. Erçağ, A. Üzer, Ş. Eren, Ş. Sağlam, H. Filik, R. Apak, Talanta 85 (2011) 2226.
- [10] N. Ular, A. Üzer Arda, S. Durmazel, E. Erçağ, R. Apak, ACS Sensors 3 (2018) 2335.

PL-04

Material History: Recent Research and New Insights into the Use of Binding Media, Meteoritic Iron and Red Lakes

Austin Nevin

University of Gotenburg, Sweden

Binding media, metals and pigments in works of art are material history - and are evidence of technology, artist practise, exchange and trade. Through the study and identification of materials, crucial data can be collected regarding physical and chemical stability thus informing conservation decisions. Three case studies of works of art and archaeological materials will draw on current research using portable instrumentation and cutting-edge analytical methods. Investigations on wall painting fragments from the ancient Canannite capital Tel Kabri allowed the identification of degraded binding media from the Aegean style wall paintings that date to the 18th C. B.C.E. The discovery of traces of organic media in the characteristic blue paint is significant for the conservation and treatment of the paintings, for understanding of the sophistication of painting practise and the use of egg-based binding media in the Eastern Mediterranean, and more broadly also questions the presence of domestic animals in the region. The second case study focuses on Tutenkhamun's dagger that was analyzed using portable instrumentation at the Egyptian Museum in Cairo. New data established conclusively that the well-conserved ornamental blade was fashioned from finely worked meteoritic iron. The identification was possible through the comparison of data acquired from the dagger with known meteor samples, and the calculation of ratios of Nickel and Cobalt. Organic red lake pigments are the focus of the third case study. Analysis demonstrates how deep crimson pigments from European insects were adopted by Leonardo in the Last Supper, and how, by contrast, Veronese adopted newly introduced Mexican pigments from cochineal insects. The molecular characterization of cross-sections demonstrate the use of similar kermes-based lakes in paintings by Leonardo and Masolino, and carmine-based reds in paintings by Tintoretto and Veronese, while also revealing soluble uncomplexed dyes in samples that has direct implications for conservation, cleaning and lighting.

PL-05

Fractional Perspectives and Quasiparticle and Excitation Energies from Ground State DFT Calculations

Weitao Yang

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The perspectives of fractional charges and fractional spins provide a clear analysis of the errors of commonly used density functional approximations (DFAs). These errors, the delocalization and static correlation error, lead to diversified problems in present-day density functional theory calculations. For achieving a universal elimination of these two errors, we develop a localized orbital scaling correction (LOSC) framework: it accurately characterizes the distributions of global and local fractional electrons and spins, and is thus capable of correcting system energy, energy derivative and electron density in a self-consistent and size-consistent manner. Our approach introduces the explicit derivative discontinuity and largely restores the flat-plane behavior of electronic energy at fractional charges and fractional spins. The LOSC-DFAs lead to systematically improved results, including the dissociation of ionic species, single bonds, multiple bonds without breaking the space or spin symmetry, the band gaps of molecules and polymer chains, the energy and density changes upon electron addition and removal, and photoemission spectra.

We further carried the comparison of experimental quasiparticle energies for many finite systems with calculations from the GW Green function and the localized orbitals scaling correction (LOSC). Extensive results with over 40 systems clearly show that LOSC orbital energies achieve slightly better accuracy than the GW calculations with little dependence on the semilocal DFA, supporting the use of LOSC DFA orbital energies to predict quasiparticle energies. This also leads to the QE-DFT (quasiparticle energies from DFT) approach: the calculations of excitation energies of the N-electron systems from the ground state DFA calculations of the (N - 1)-electron systems. Results show good performance with accuracy similar to TDDFT and the delta SCF approach for valence excitations with commonly used DFAs with or without LOSC. For charge transfer and Rydberg states, good accuracy was obtained only with the use of LOSC DFA. The QE-DFT method has been further developed to describe excited-state potential energy surfaces (PESs), conical intersections, and the analytical gradients of excited-state PESs.

- [1] J. Cohen, P. Mori-Sanchez, and W. Yang. *Science*, 321:792, 2008.
- [2] P. Mori-Sánchez, A. J. Cohen, and W. Yang, *Physical Review Letters*, 100: 146401, 2008.
- [3] P. Mori-Sanchez, A. J. Cohen, and W. Yang. *Physical Review Letters*, 102:066403, 2009.
- [4] J. Cohen, P. Mori-Sanchez, and W. Yang. *Chem. Rev.* 112:289, 2012.
- [5] C. Li, X. Zheng, N. Q. Su, and W. Yang, *National Science Review*, 5: 203–215, 2018.
- [6] N. Q. Su, C. Li, and W. Yang, *Proceedings of the National Academy of Sciences*, 115:9678–9683, 2018.

- [7] Y. Mei, C. Li, N. Q. Su, and W. Yang *arXiv:1810.09906* 2018; *J. Phys. Chem. A*, 123(3), 666–673, 2019.
[8] Y. Mei and W. Yang, *J. Chem. Phys.*, 150, 144109, 2019.
[9] Y. Mei and W. Yang, *J. Phys. Chem. Lett.* 10, 2538–2545, 2019.

PL-06

In-Situ TEM Studies of Biomineralization

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This talk will provide an overview of the PIs' efforts to understand the dynamics of biomineralization via in-situ transmission electron microscopy. First, we demonstrate how to utilize graphene sheets to build a liquid-cell nanoreactor that fits the chamber of high-resolution TEM. Graphene is impermeable to liquids such as aqueous solutions and therefore can be used to seal liquid solutions from leaking to the high vacuum of TEM environment. In addition, the excellent electrical conductivity of graphene and its ability to scavenge the radicals produced by the interaction of electron beam and liquid solutions provide an excellent platform to perform imaging of biological or hydrated specimens.

We then demonstrate our success to observe the biomineralization of hydroxyapatite (HA) crystals. Our results show that HA crystals follow classical and non-classical nucleation theories to form within a supersaturated solution. The solution initially goes through ion-rich and ion-poor liquid-liquid phase separation. Amorphous calcium phosphate (ACP) acts as template for the biomineralization of HA while HA can also form by aggregation of primary HA nanoparticles.

We also studied the effect of molecular modifiers on the effect of calcium oxalate crystals that are the primary constituent of kidney stones. We show that the addition of citrate can affect the crystallization pathway of these minerals. Interestingly, the citrate molecules affect the pre-nucleation stage of CaOx crystals making them thermodynamically stable. In addition, the addition of citrate reduces the stability of calcium oxalate monohydrates.

In addition, we will showcase some examples of biomineralization of iron oxide core in ferritin proteins and demonstrate the ability to monitor the biomineralization of these crystals using graphene liquid cells in TEM. We will show that the ratio of L and H subunits in the ferritin protein shells can affect the nucleation and growth of iron oxide cores.

We also will present our latest results on the biomineralization of magnetosomes in magnetotactic bacteria grown in iron-rich media using in situ GLC-TEM studies. We observed that such bacteria can remain alive and intact during TEM imaging and follows the classical nucleation theory for the biomineralization of magnetosomes.

PL-07

Two-Dimensional Materials and 3D Printing of Li Batteries

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Design of safe lithium ion batteries require innovations in manufacturing, characterization, modeling and simulation, and development of new materials. This presentation provides an overview on the efforts in the PI's lab to design thermally safe and high energy density batteries. We demonstrate the shortages and gaps in the field of lithium ion batteries that require advanced characterization. In particular we show that in-situ transmission electron microscopy (TEM) is fundamental to discover mechanisms of ion conductivity, structural degradation and transformations, and other structural phenomena associated with the behavior of electrodes. In addition, we show that additive manufacturing such as 3D printing hold a great potential to fabricate the next generation battery devices.

PL-08

Drug Delivery Systems for Optimizing the Therapeutic Index

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Drugs have to overcome many barriers in order to reach their target. In specific, highly lipophilic drugs suffer from low solubility and bioavailability and therefore fail to reach the target. Furthermore, they produce undesired metabolic products and reach fault targets. Therefore, the use of nanopharmacology technology has provided new formulations, to overcome these undesired properties. Specifically, vehicles such as cyclodextrins and calixarenes, micelles and liposomes have been used to host highly lipophilic drugs such as AT1 antagonists, quercetin and silibinin. The encapsulation of these drugs in supramolecules or other systems leads to their solubility optimization and metabolic stability. In addition, the drug is aided to reach only the specific target, decrease the effective dose and improve the therapeutic index.

Examples will be given from our research activity that prove the significance of supramolecules in rational drug design. The complexing of quercetin in calixarene and finally the forming of nanoparticle resulted in increasing of its solubility and bioavailability properties and specific effects on cancer cells. The same results have been observed when silibinin was engulfed in cyclodextrin. Improvement in solubility and in vitro results have been also observed with the AT1 antagonist irbesartan. Interestingly, when irbesartan is embedded in liposomes forms some crystals which prohibit its full effectiveness in perturbation. However, when the drug is hosted by 2-hydroxypropyl- β -cyclodextrin is released completely in the core of the liposomes and exerts full perturbing action.

The above experimental evidence points out that improvement can be achieved by drug delivery through the use of supramolecules and the knowledge of the molecular basis of action can be enhanced. This is a valuable information if rational design must be applied using nanotechnology formulations.

PL-09

Nondifferentiated and Differentiated Stony Meteorites: Comparative Analysis Using X-Ray Diffraction, Magnetization Measurements and Mössbauer Spectroscopy

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Nondifferentiated stony meteorites are mainly ordinary chondrites. These meteorites have the age comparable with the age of Solar System. Ordinary chondrites consist of various iron-bearing crystals such as olivine (Fe, Mg)₂SiO₄, orthopyroxene (Fe, Mg)SiO₃, clinopyroxene (Fe, Mg, Ca)SiO₃, troilite FeS, chromite FeCr₂O₄, hercynite FeAl₂O₄, ilmenite FeTiO₃ as well as grains of Fe-Ni-Co alloy in the form of η -Fe(Ni, Co), η 2-Fe(Ni, Co), η -Fe(Ni, Co) and η -FeNi phases. Differentiated stony meteorites (achondrites) are the result of asteroids and protoplanets differentiation with formation of iron alloy core and stony shell. These meteorites may consist of pyroxenes mainly with troilite, chromite, ilmenite, etc.

In the present work we present a comparison of the results of the studies of some ordinary chondrites and one achondrite (howardite) using X-ray diffraction, magnetization measurements and Mössbauer spectroscopy. The observed differences are discussed considering the possible effect of matter differentiation.

Keywords: Stony meteorites; X-ray diffraction; Magnetization measurements; Mössbauer spectroscopy.

Acknowledgements

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TURCMOS 2019



Oral Abstracts

O-01

Characterization of Proteins by Vibrational Spectroscopy

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Antibodies are one of the top biopharmaceuticals market type due to their applications in oncology therapy. However, they can undergo changes at different structural levels that can result in loss of their activity [1]. Although mass spectrometry is a powerful technique for primary structure determination, it fails to give information at higher order levels. In this project we explored the possibilities of vibrational spectroscopic techniques as a tool kit to help ensure the integrity and batch to batch reproducibility in antibody manufacture.

Infrared (IR) and Raman spectra are well known to contain bands (Amide I, II and III) with shapes that correlate to secondary structure (SS) [2][3][4]. Unlike Circular Dichroism (CD) (the most well-established technique for secondary structure analysis [5]), IR and Raman spectroscopy allow much wider ranges of optical density which makes the analysis of complex pharmaceutical samples more feasible. However, the data processing and extraction of this information are ambiguous and, in many cases, limited by spectral noise and water absorption in IR and fluorescence in Raman. A neural network algorithm that we called self-organizing maps (SOMspec) was implemented for the prediction of SS by fitting the Amide I with a reference set of proteins of known SS. Data sets of proteins were collected in both solid and aqueous state by Raman, IR and Raman Optical Activity. The proteins used for the experiments were commercial ones with the highest possible SS coverage. The results presented in figure 1 correspond to those of solid state by Raman. Although in general pretty accurate, for some of the proteins the predictions were far from expected meaning the reference sets might not be large enough or the shape of the bands are not always univocal to SS as thought. Complementary analysis of the Amides II and III are to be performed in the near future.

Keywords: Proteins; Secondary structure; Raman; Infrared; Neural network.

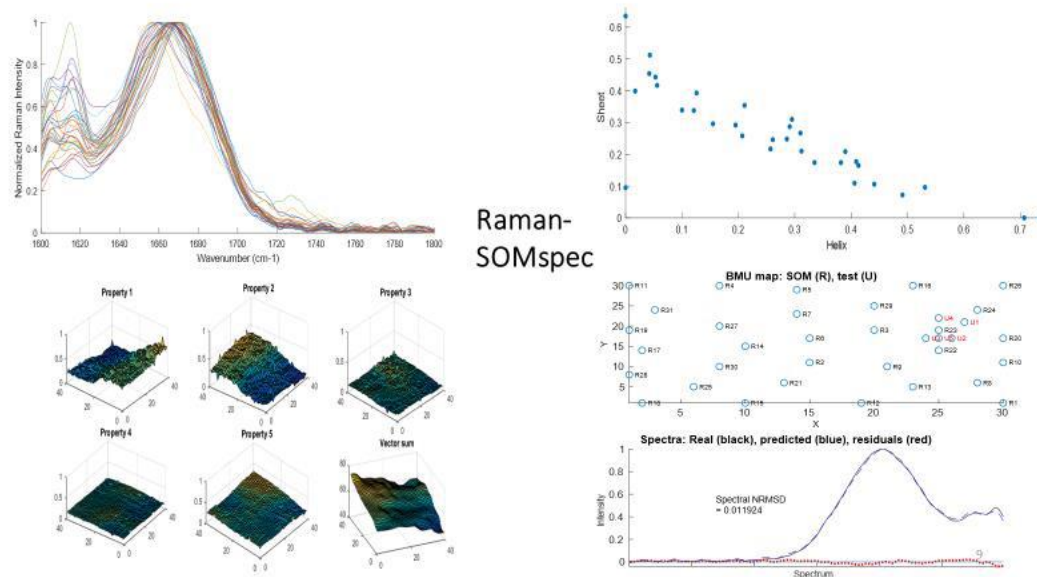
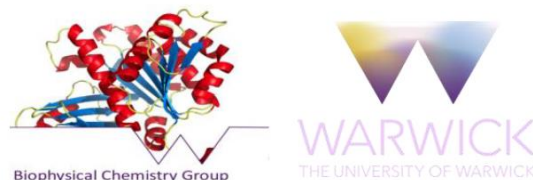


Figure 1. Raman reference set (upper-left), coverage of helical and beta strand structures (upper-right), SOM map and fitted protein (lower-right) and distribution of properties on the map (lower-left).

Acknowledgements



- [1] S. Ausar, Hasija, Li, and Rahman, "Forced degradation studies: an essential tool for the formulation development of vaccines," *Vaccine Dev. Ther.*, 2013, pp. 11.
- [2] J. Kong and S. Yu, "Fourier Transform Infrared Spectroscopic Analysis of Protein Secondary Structures Protein FTIR Data Analysis and Band Assignment," vol. 39, no. 8, 2007, pp. 549–559.
- [3] A. Barth, "Infrared spectroscopy of proteins," vol. 1767, 2007, pp. 1073–1101.
- [4] A. Rygula, K. Majzner, K. M. Marzec, A. Kaczor, and M. Pilarczyk, "Raman spectroscopy of proteins : a review," no. July, 2013, pp. 1061–1076.
- [5] S. M. Kelly, T. J. Jess, and N. C. Price, "How to study proteins by circular dichroism," vol. 1751, 2005, pp. 119–139.

O-02

Development of a Spatially Offset Raman Spectroscopy Method for non-invasive Assessment of Bone Quality

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Age and disease-related low trauma bone fractures have a growing economic burden along with reducing the life quality of the patients [1]. Such fractures can further cause morbidity and even mortality especially among elderly people [2]. The best strategy dealing with bone fracture is to prevent the fracture. Bone Mineral Density (BMD)-based fracture risk assessment is currently gold standard, but not sufficient enough to robustly predict bone fracture risk since bone fracture resistance originates from bone mass, bone architectural/structural properties and bone matrix/material quality [3]. Though several clinical measurements (Dual-energy X-ray absorptiometry (DXA), peripheral quantitative computed tomography (HR-pQCT), micro-magnetic resonance imaging (μ MRI) and Ultrasound) provide meaningful clinical assessment of bone mass and bone architectural/structural properties [4], a barrier to establishing a robust, patient-specific fracture risk assessment is the lack of a diagnostic tool that is sensitive to the bone matrix quality. Being both sensitive to composition and organization of all three primary components of bone (mineral, organic matrix, and water), Raman spectroscopy holds a great potential to assess bone matrix quality with the advantage of its clinical feasibility in the near term. Herein, using a cadaveric human tibia and chicken meat slices (1 mm thickness) to simulate the bone covered by layered soft tissues in human body, a phantom study was conducted to demonstrate the feasibility of using spatially offset Raman spectroscopy (SORS) with customized Raman probes to collect Raman bone spectrum beneath the layered soft tissues. The results showed that Raman bone spectrum can be collected up to 1 cm depth transcutaneously through creating 8 to 20 mm offset between laser exposure fiber and laser collection fibers. With further optimization in this technique combining with current clinical measures, a patient-specific robust bone fracture risk assessment could be fully realized in the near future.

Keywords: Raman spectroscopy; Bone; Fracture Risk; SORS.

Acknowledgements

The author sincerely thanks to Prof. Dr. Anita Mahadevan-Jansen and Assoc. Prof. Dr. Jeffry S. Nyman for providing valuable technical support and the SORS equipment during data collection of this study.

[1] O Johnell et al., *Osteoporos Int*, 2006 17:1726.

[2] Cynthia L. Leibson et al. *J Am Geriatr Soc*, 2002 50:1644.

[3] Mustafa Unal et al., *Curr Osteoporos Rep*, 16(3), 2018, 205-215.

[4] Eve Donnelly, *Clin Orthop Relat Res*, 469(8), 2011, 2128-2138.

O-03

**Investigation of the Effect of A-Lipoic Acid on Liver Cell Damage
in Acitretin and Methotrexate Given Rats**

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In this study, the effect of α -Lipoic Acid (ALA) on liver cell damage in Acitretin (ACT) and Methotrexate (MTX) treated rats was researched. ACT, which has been used for many years, has been used in combination with MTX in recent years. Although this combination is effective in the treatment of some diseases, it has been shown to have serious side effects on the liver and other organs. The aim of this study was to determine the benefits of antioxidant ALA in eliminating the cellular damage caused by free radicals produced by ACT and MTX. In our study, a total of 50 Wistar albino male adult rats weighing between 200 and 250 g were used. At the same time, these rats were selected from the same generation. The rats were fed with standard mouse food and water was given free.

Keywords: Malondialdehyde; Acitretin; Methotrexate; Liver.

[1] H.H. Draper and M. Hadley, Malondialdehyde determination as index of lipid peroxidation, 186, 1990, 421–431.

[2] Maritima A. C., Sanders R. A., Watkins J. B. Effects of lipoic acid on biomarkers of oxidative stress in streptozotocin-induced diabetic rats. *Journal of Nutritional Biochemistry*, 2003, 14, 288–294.

[3] Jingang Ana, Dingwei Zhanga, Jiawen Wua, Jiong Lib, Xiu Tengb, Xiaomin Gaoa, Ruilian Lia, Xiuying Wanga, Linlin Xiac, Yumin Xiaa,* The acitretin and methotrexate combination therapy for psoriasis vulgaris achieves higher effectiveness and less liver fibrosis, *Pharmacological Research*, 2017, 121, 158–168.

O-04

Biosynthesis and Characterization of Gold Nanoparticles using *Persea Americana* Leaf Extract

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This study aims to examine the reducing potential of *P. americana* leaf extract for the synthesis of gold nanoparticles (AuNPs). The AuNPs were synthesized and characterized with different spectroscopic techniques. The formation of AuNPs was confirmed by color change and Ultraviolet-visible spectroscopic analysis. Nanoparticles exhibited surface plasmon resonance at 532 nm. The phytoconstituents involved in the reduction and stabilization of AuNPs were identified using fourier transform infrared spectra.

As is known, the stability of nanoparticles plays an important role, especially in biological applications. The reduction in particle stability may significantly alter their cellular uptake and toxicity. For this purpose, the effects of different volumes of 0.1 M NaCl starting from 1 mL to 50 μ L were used to test particle stability. The results showed that the nanoparticles synthesized using *P. americana* leaf extract were extremely stable even in different volumes of NaCl levels. Colloidal stability of the nanoparticles in the presence of strong ionic strength was also confirmed by colorimetric observations.

These results suggest that *P. americana* leaf extract can be used as reducing agent for the synthesis of AuNPs. Biosynthesized AuNPs showed enhanced colloidal stability, making them suitable for biomedical applications.

Keywords: Green synthesis; Gold nanoparticles; *Persea americana*; Colloidal stability.

O-05

Diabetes Induces Structural Alterations in Proteins and Lipids in Kidney Glomeruli

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Diabetes Mellitus (DM) is a destructive metabolic disorder characterized by abnormally high blood glucose levels due to decreased secretion or effectiveness in function of insulin. The complications of DM lead to chronic, irreversible damages to vital organs and systems including diabetic nephropathy. This study aims to investigate the structural and compositional alterations in the glomeruli of diabetic rat kidneys. Adult male Wistar rats were randomly divided into two groups as control and diabetic. Diabetes was induced by a single intraperitoneal injection of STZ (50mg/kg), and 3 days after the STZ injection the rats having hyperglycemia (>300 mg/dl) were assigned to be diabetic. The animals were maintained for 6 weeks for the progression of diabetic nephropathy. Kidneys were embedded into paraffin, 10 µm thick cross-sections were transferred onto BaF2 windows, deparaffinized and spectral maps of glomeruli were collected by Fourier transform infrared (FTIR) imaging. The spectral maps were then analyzed utilizing band area and intensity ratios by Isys software. Moreover, extracted spectra were evaluated by neural networks in order to depict protein structural alterations. The results revealed that 1338 cm⁻¹/Amide II band area ratio, which can be used to monitor the collagen integrity [1], and the band intensity ratio of 1660 cm⁻¹/1690 cm⁻¹, which reveals collagen maturity and structural alterations in collagen [1,2], were observed to be decreased in diabetic kidneys. These findings indicate a structural change in the collagen and the helical integrity of collagen is decreased in diabetic glomeruli. The neural network analysis of protein secondary structures further indicated that the amount of α-helices and β-turns were decreased whereas the amount of β-sheet and random coil structures were increased in diabetic kidneys. Moreover, the results of the CH₂ antisymmetric stretching/ CH band area ratio revealed that diabetes led to a decrease in saturated lipid content in diabetic glomerulus membranes, which indicates a decrease in the hydrocarbon chain length in lipid structure [3]. In addition, a decrease in the unsaturated lipids in diabetic glomeruli was also observed by the monitoring of the olefinic/CH and olefinic/CH₂ antisymmetric stretching band area ratios. This result demonstrates the lipid peroxidation in diabetic glomeruli membranes. In conclusion, the results revealed the structural alterations in lipids and proteins in diabetic glomeruli, especially in collagen structure.

Keywords: Diabetes; Kidney; Collagen; FTIR imaging; Neural network analysis.

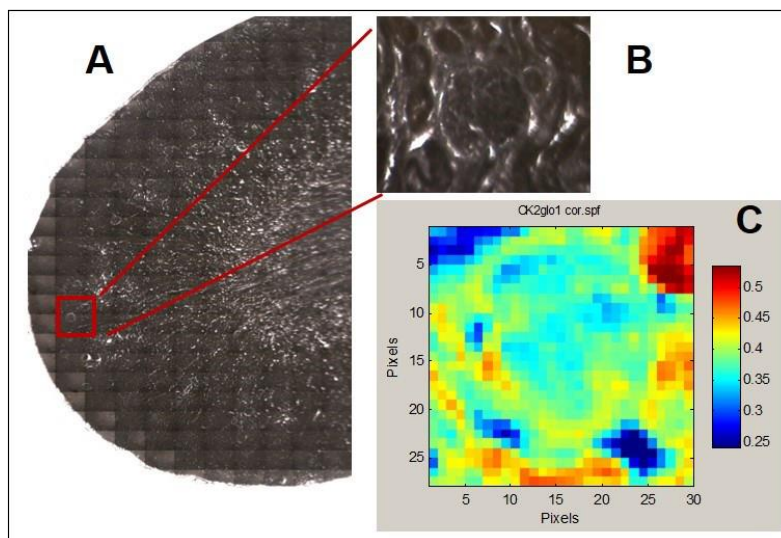


Figure 1. A) The visible image of a control kidney section, B) The visible image of the glomerulus marked in A, C) The total absorbance FTIR image of the glomerulus.

Acknowledgements

The authors would like to thank to Prof. Dr. Feride Severcan for providing laboratory facilities.

- [1] A. Hanifi, J.B. Richardson, J.H. Kuiper, S. Roberts, N. Pleshko, *Osteoarthritis Cartilage*, 20, 9, 2012, 988-996.
- [2] R.Y. Huang, L.M. Miller, C.S. Carlson, M.R. Chance, *Bone*, 33, 4, 2003, 514-521.
- [3] G. Cakmak, L.M. Miller, F. Zorlu, F. Severcan, *Archives of Biochemistry and Biophysics*, 520, 2012, 67-73.

O-06

Synthesis, Spectroscopic, Thermal, and Structural Properties of Three New Bimetallic Cyano-bridged Coordination Polymers Containing 4-aminomethylpyridine

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Three new bimetallic cyano-bridged coordination polymers with chemical formulas $[\text{Fe}(\text{NH}_3)_2(\text{ampy})\text{Ni}(\text{CN})_4]_n$ (**1**), $[\text{Co}(\text{H}_2\text{O})_2(\text{ampy})\text{Ni}(\text{CN})_4]_n$ (**2**) and $[\text{Ni}(\text{NH}_3)_2(\text{ampy})\text{Ni}(\text{CN})_4]_n$ (**3**) (ampy = 4-aminomethylpyridine) were synthesized in the form of powders and examined by vibrational (infrared and Raman) spectroscopy, thermal (TG, DTG and DTA) and elemental analysis techniques. The FT-IR and Raman spectra of the complexes were performed in the range of $4000\text{--}400\text{ cm}^{-1}$ and $4000\text{--}250\text{ cm}^{-1}$, respectively. Considering the variations in the vibrational frequencies of the cyano group and ampy ligand in the spectrum of the complexes, the Ni(II) atom is a square plane geometry with four cyano groups and two of these cyano groups are bridge and the other two are terminal. In addition, the metal atoms [Fe(II), Co(II) or Ni(II)] are connected by the ring and amino nitrogen atoms of two symmetric ampy ligands, the two ammine [two aqua ligands for (2)] ligands and the two bridging cyano groups and show a distorted octahedral geometry. The spectral properties revealed that the structures of the complexes consist of 2D networks. Similar structural properties were observed in the complexes $[\text{Cu}(\text{NH}_3)_2(\mu\text{-ampy})\text{M}(\mu\text{-CN})_2(\text{CN})_2]_n$ [ampy = 4-aminomethylpyridine, M = Ni(II), Pd(II) and Pt(II)] [1]. Thermal stabilities and decomposition products of these complexes were also investigated in the temperature range of $30\text{--}700\text{ }^\circ\text{C}$ using TG, DTG and DTA techniques in the static air atmosphere.

Keywords: Tetracyanonickelate; 4-aminomethylpyridine; Vibration spectra; Thermal analysis.

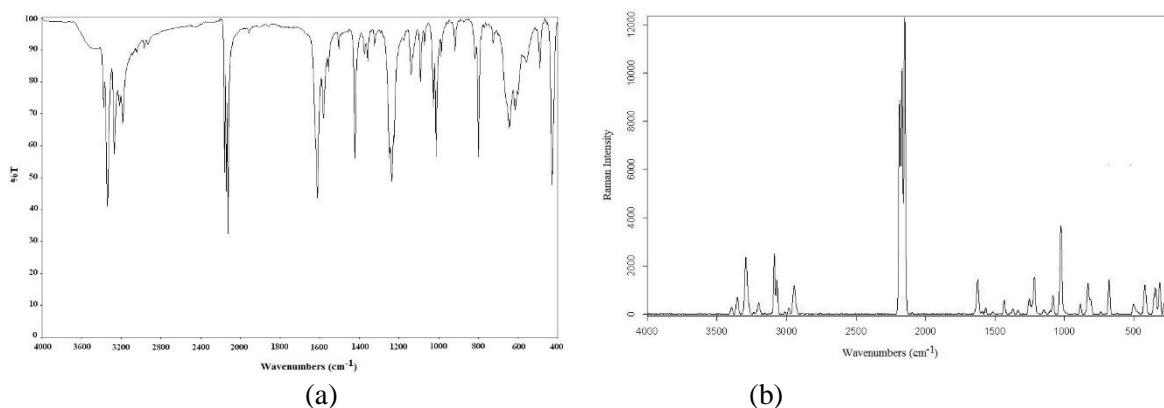


Figure 1. The FT-IR (a) and Raman (b) spectrum of **1**.

[1] D. Karaağaç, G.S. Kürçüoğlu, O.Z. Yeşilel, T. Hökelek, Spectrochim. Acta, Part A.; 121, 2014, 196-204.

O-07

Green Synthesis, Characterization of Gold Nanoparticles using the Aqueous Extract of *Russula delica*.

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Metal nanoparticles are used in the medical industry, food packaging, bioengineering, catalysis and environmental science applications. However, the observed in vitro and in vivo toxicity leads to significant difficulties in the synthesis and application of metal nanoparticles. The fact that the nanoparticles synthesized chemically contain toxic chemicals that can pollute the environment and cause harm to animals, has led to the development of green nanotechnology which combines biological principles with physical and chemical procedures.

Compared to other naturally available biological sources, fungi are more efficient, so they are more suitable for the synthesis of nanoscale metal particles. It produces large amounts of protein that contribute to the high productivity and stability of particles that are easy to use and fabricate. In addition, fungal micelles can withstand environments in bioreactors.

The aim of this study was to make easy and economical synthesis of gold nanoparticles (AuNPs) using *Russula delica* (RD) mushroom extract, which shows bioactive properties such as antioxidant, anticancer and antimicrobial. Characterization of RD-AuNP UV-Visible Spectrophotometer (UV-Vis.), XRD (X-ray crystallography), SEM (Scanning electron microscopy), FT-IR (Fourier transform infrared Spectroscopy), EDAX (Energy Dispersed X-Ray Spectrum), TGA-DTA (Thermal Gravimetric Analysis). RD-AuNPs synthesized have a crystal size of 80 nm in the spherical appearance. As a result, fungal systems used for nanomaterial biosynthesis as an effective alternative to chemical synthesis can be used in different biotechnological and medical applications. RD-AuNPs produced by green synthesis can be evaluated in this context.

Keywords: AuNPs; Fungus; SEM; UV-Vis; XRD.

O-08

Photoluminescence of Mn⁴⁺ Activated Li₂TiO₃: The Route for Highly-sensitive Luminescence Thermometry

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Photoluminescence of Mn⁴⁺ activated lithium metatitanate (Li₂TiO₃) powders exhibits intense deep-red emission (centered around 688 nm) from the Mn⁴⁺ 2E_g → 4A_{2g} spin forbidden transition. Herein, we demonstrate that optical properties of this material are suitable for both luminescence thermometry [1] and the fabrication of phosphor converted LEDs for artificial plant growth. Structural analysis shows that Mn⁴⁺ ions are equally distributed in two almost identical Ti⁴⁺ sites in which they are octahedrally coordinated by six oxygen ions. Calculations based on the exchange charge model of the crystal field provided values of Racah parameters (B=760 cm⁻¹, C= 2993 cm⁻¹), crystal-field splitting Dq= 2043 cm⁻¹, and the nephelauxetic parameter β₁=0.9775, while calculated energy levels are in good agreement with the measured excitation and luminescence spectra. Maximal quantum efficiency of 24.1% at room temperature is found for 0.126% Mn⁴⁺ concentration which is quite high value considering that Mn⁴⁺ emission is already temperature-quenched at room temperature. For larger Mn⁴⁺ concentrations, emission decreases in intensity as a result of a non-radiative energy transfer between Mn⁴⁺ ions which is facilitated by electric dipole-dipole interactions. Temperature quenching of emission occurs by a cross-over via 4T₂ excited state of the Mn⁴⁺ ions with T_{1/2} = 262K. Temperature induced quenching of Mn⁴⁺ emission in Li₂TiO₃ is quite favorable for the application in the lifetime-based luminescence thermometry since relative changes in emission decay values are significant in the temperature range from 50 to 225K, and exceptionally-large for higher temperatures where they reach 3.21% (around room-temperature). We derived theoretical expressions for the temperature dependence of the absolute and relative lifetime sensitivities of Mn⁴⁺ activated materials, and present detailed discussion on the influence of host material properties on lifetime sensitivities. It is shown that the hosts with low values of the energy of phonon coupling to the 2E_g → 4A_{2g} transition and cross-over energy are favorable for the lifetime-based luminescent thermometry at low temperatures, while hosts with large values of these energies should be used for the high-temperature thermometry. The discussion on engineering of the Mn⁴⁺ activated materials for high-precision luminescence thermometry via the control of the 4T_{2g} level and phonon coupling energies is given at the end of paper.

Keywords: Mn⁴⁺ emission; Luminescence thermometry; Photoluminescence quenching.

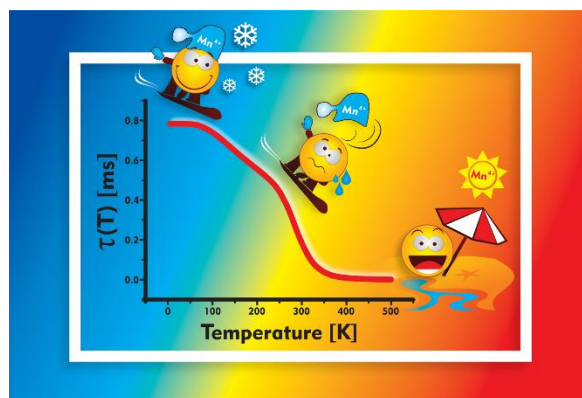


Figure 1. Emission decay times of Mn^{4+} activated Li_2TiO_3 deep-red phosphor can be used for the high-performance temperature sensing with temperature resolution better than 30 mK.

Acknowledgements

Authors acknowledge the funding from European Union project “NanoTBTech – Nanoparticles-based 2D thermal bioimaging technologies” (H2020-FETOPEN-1-2016-2017, Grant: 801305).

[1] Miroslav Dramićanin, *Luminescence Thermometry: Methods, Materials, and Applications*, Woodhead Publishing, 2018.

O-09

Discrimination of Cancer Cell Subpopulations based on FTIR Spectral Data

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A small subpopulation of tumor cells called 'stem cell-like cells' (or cancer stem cells, CSCs) lead to chemotherapy/radiotherapy resistance, relapse and metastasis. The aim of the present study is to discriminate the cancer cell subpopulations based on the spectral data of cellular biochemical features in order to understand the molecular mechanism of CSCs further and to find out therapeutic biomarker against CSCs if any. Fourier transform infrared (FTIR) spectroscopy has been extensively used to analyze biological samples, providing rapid information on the composition, concentration and structure of cellular macromolecules (lipids, proteins, carbohydrates and nucleic acids) [1–4]. As methodology, in human breast cancer, the cells with CD44+/CD24– markers were isolated from MCF-7 cell line by using flow cytometry. Attenuated total reflection (ATR)-FTIR spectroscopy was used to record the cell spectra of dehydrated samples in the fingerprint region of 4000–800 cm⁻¹. Spectral preprocessing, partial least squares-discriminant analysis (PLS-DA), principal component analysis and hierarchical cluster analysis were carried out with software 'Kinetics'. The results indicated that the IR-based assay was capable of classifying the cell subpopulations based on the variations in biochemical features in CSCs. Multivariate statistical analysis revealed that CSCs was successfully discriminated both from breast cancer cells and breast healthy cells. In conclusion, this approach provides rapid and accurate discrimination between cell subpopulations based on the cell specific patterns and can be used in a variety of fields.

Keywords: FTIR spectroscopy; Discrimination; Cancer stem cell; Multivariate statistical analysis.

Acknowledgements

We are grateful to Prof. Dr. Ercüment Karasulu (ARGEFAR, Ege University) for his permission for the usage of FTIR spectrometer. We thank Prof. Dr. Huseyin Aktug and Prof. Dr. Gulperi Oktem for providing the cell lines. We thank to Prof. Dr. Erik Goormaghtigh from Université libre de Bruxelles, Belgium for providing the software 'Kinetics'.

[1] M. Diem, S. Boydston-White, L. Chiriboga, *Appl. Spectrosc.* 53 (1999) 148A–161A.

[2] G. Güler, U. Guven, G. Oktem, *Analyst.* 144 (2019) 2138–2149.

[3] G. Güler, E. Acikgoz, N.Ü. Karabay Yavasoglu, B. Bakan, E. Goormaghtigh, H. Aktug, *Analyst.* 143 (2018) 1624–1634.

[4] E. Acikgoz, G. Güler, M. Camlar, G. Oktem, H. Aktug, *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* 209 (2019) 150–164.

O-10

Investigation of Large-Area MoSe₂ Monolayer Formation using NaCl Salt Catalyzer by Raman Scattering and Photoluminescence Spectroscopy

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Monolayer MoSe₂, a member of 2D two dimensional transition metal dichalcogenide (TMDs) family has attracted considerable attention due to its direct bandgap and high mobility suitable for both optoelectronic and electronic devices [1]. However, to produce uniform and large-area MoSe₂ monolayer structures over the whole substrate with a high coverage is still a challenging issue due to the difficulty in controlling the growth of single-layer structures [2, 3]. Using glass as a substrate is reported to be favorable in chemical vapor deposition (CVD) reactions, extending the lateral growth of monolayer MoSe₂ [3, 4]. However, there are several issues to be clarified regarding the role of a glass substrate in monolayer formation. For example, it is not fully understood whether the glass surface reactions or glass impurities such as Na, Mg, Ca and etc. function as a catalyzer or supporter to produce homogeneous, large-area and monolayer MoSe₂ flakes. Hence, in this study, we report the synthesis and characterization of monolayer MoSe₂ structures formed on 300 nm SiO₂ coated Si substrate where NaCl salt is used as a catalyzer in CVD process. We have also fabricated and compared the electronic properties of a back-gate field effect transistors (FET) based on these salts induced flakes and conventionally CVD grown MoSe₂ flakes. 0.05 molar NaCl solution is dropped and spinned on a SiO₂/Si substrate (4 cm x 4 cm) by 500 rpm for 120 seconds. After the spinning process, the substrate is kept for 120 seconds on a hot plate (70 °C) as shown in Figure 1 a). Molybdenum trioxide (MoO₃), selenium (Se) powders, and NaCl coated substrate are placed on a quartz tube in the CVD chamber. CVD reactions take place under ambient pressure conditions with a temperature ramping rate of 20 °C min⁻¹ where the growth temperature is 850 °C and reaction period is 5-minutes. Single layer MoSe₂ flakes with a thickness of ~0.70 nm and a lateral dimension up to 100 μm are uniformly produced. Raman spectroscopy, photoluminescence (PL) spectroscopy, atomic force microscopy (AFM) and optical microscopy are used for characterizing the formed structures. The photoluminescence peak of A exciton emission of NaCl salt assisted MoSe₂ is observed at 812 nm and Raman peak, out of plane mode (A¹_g) observed at 238 cm⁻¹ is assigned to monolayer MoSe₂ flake formations shown in figure 1 b) and c). Photoluminescence peak of A exciton emission of MoSe₂ grown on glass substrate is observed at 812 nm and Raman peaks observed at 270 cm⁻¹ (E¹_{2g}), 238 cm⁻¹ (A¹_g), 220 cm⁻¹ (E¹_{1g}) shown in figure 1 d) and e). Optical measurements performed by both bright field and dark field microscopy to show grain boundaries, uniform growth and the obtained sizes of the salt assisted grown MoSe₂ flakes and MoSe₂ flakes grown on glass substrates are shown in figure 2. In conclusion, NaCl involvement in CVD process enables large area MoSe₂ flakes with full substrate coverage, which was not possible with process without any salt [5]. Hence, we confirm that NaCl develops CVD kinetics via reducing strength of

interlayer bonds of MoSe₂ flakes and enlarges homogeneous, laterally grown monolayer device-quality MoSe₂ flakes, which is crucial for practical applications of 2D TMDCs.

Keywords: CVD; MoSe₂; FET; Raman scattering spectroscopy; Photoluminescence.

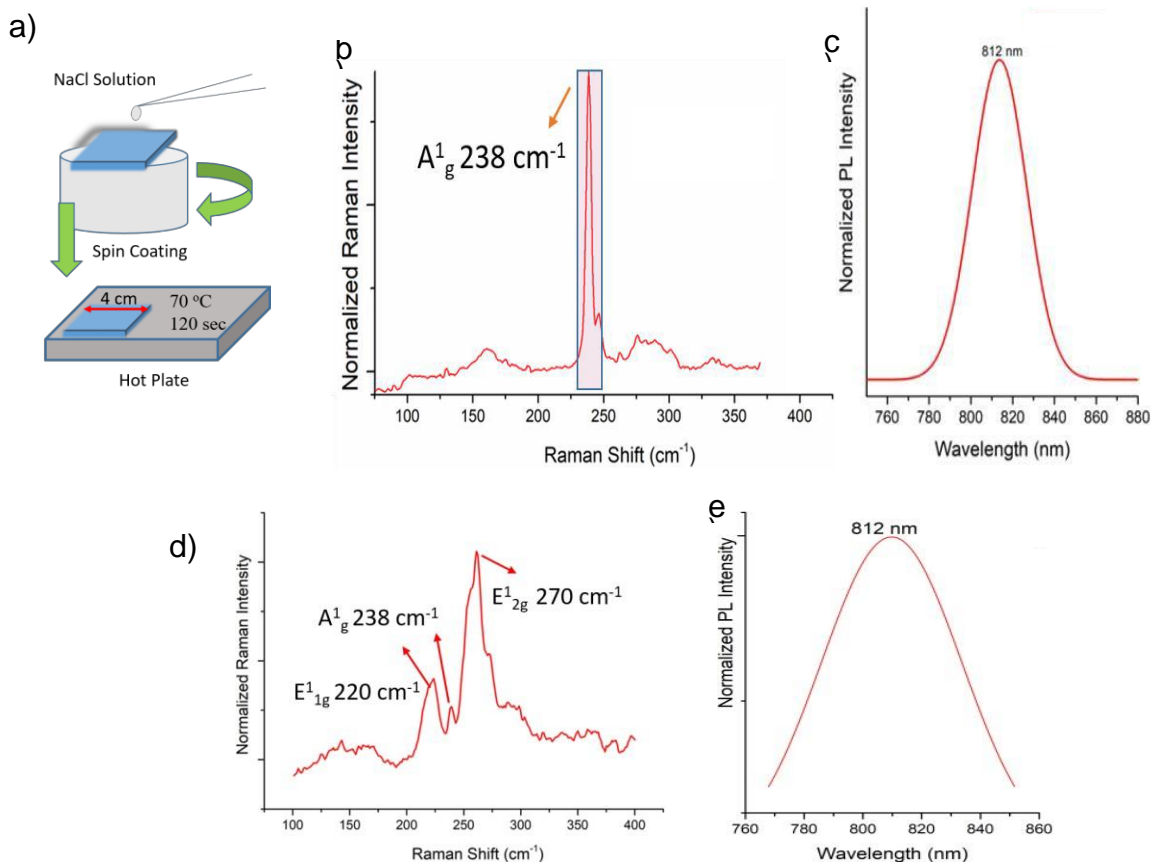


Figure 1. a) The process schematics of substrate coating by NaCl solution b) Raman shift spectra of NaCl assisted MoSe₂ flakes c) Photoluminescence (PL) measurement of MoSe₂ flakes grown by NaCl assistance d) Raman scattering spectra of MoSe₂ flakes grown on glass substrate e) Photoluminescence (PL) measurement of MoSe₂ flakes grown on glass substrate.

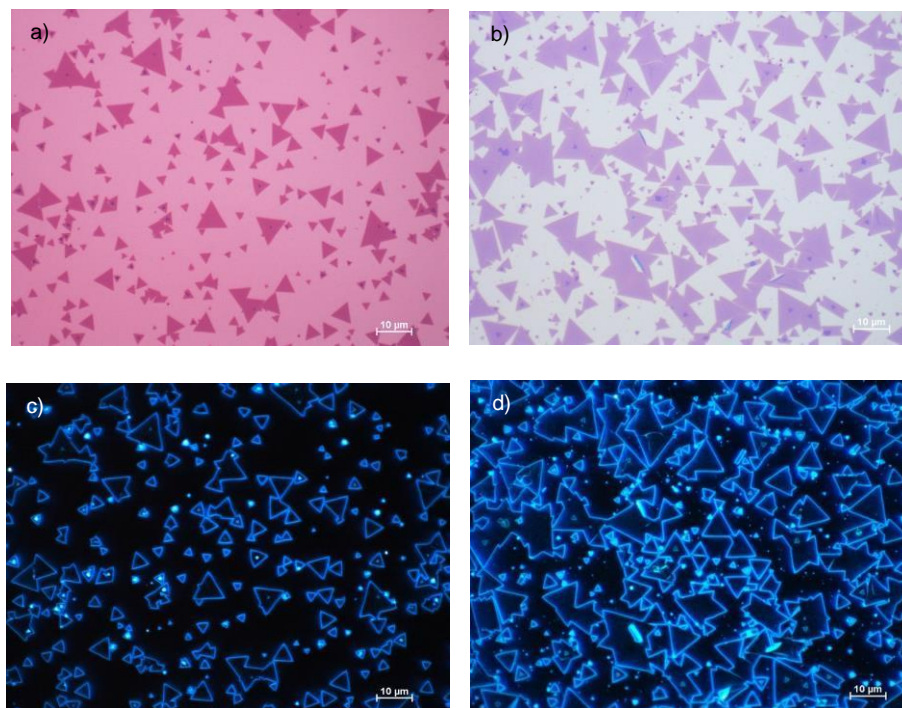


Figure 2. a) Bright field (BF) optical measurement of NaCl assisted MoSe₂ flakes b) Bright field (BF) optical measurement of MoSe₂ flakes grown on glass substrate c) Dark field (DF) optical measurement of NaCl assisted MoSe₂ flakes d) Bright field (BF) optical measurement of MoSe₂ flakes grown on glass substrate.

Acknowledgements

This work was supported by Eskişehir Technical University research projects no: BAP1804F085.

- [1] P. Nihan Kosku, B. Mehmet, Investigation of Single-Wall MoS₂ Monolayer Flakes Grown by Chemical Vapor Deposition, *Nano-Micro Letters*, 8 (2015).
- [2] H.O. Pierson, 2 - Fundamentals of Chemical Vapor Deposition, *Handbook of Chemical Vapor Deposition (CVD) (Second Edition)*, William Andrew Publishing, Norwich, NY, 1999, pp. 36-67.
- [3] H.O. Pierson, 3 - The Chemistry of CVD, *Handbook of Chemical Vapor Deposition (CVD) (Second Edition)*, William Andrew Publishing, Norwich, NY, 1999, pp. 68-83.
- [4] W. Zhan, X. Yong, W. Haolin, W. Ruixue, N. Tang, Z. Yongjie, S. Jing, J. Teng, Z. Ying, L. Yimin, Y. Mei, W. Weidong, Z. Qing, M. Xiaohua, H. Yue, NaCl-assisted one-step growth of MoS₂ -WS₂ in-plane heterostructures, *Nanotechnology*, 28 (2017) 325602.
- [5] M. Bay, A. Özden, F. Ay, N.K. Perkgöz, Bandgap tuning of Monolayer MoS₂(1-x)Se_{2x} alloys by optimizing parameters, *Materials Science in Semiconductor Processing*, 99 (2019) 134 - 139.

O-11

A New, Simple and Green Switchable Solvent Extraction of Rhodamine B and its Spectrophotometric Determination in Water, Food and Soft Drink Samples

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Rhodamine B is widely used in industrial process such as printing and dyeing in textile, paper, paints, leathers, etc. However, the organic dyes will cause serious environmental and biological problems, even capable to induce irritation to the skin, eyes [1]. So, determination of rhodamine B in water, food and environmental samples is very important for human and animal health. Direct determination of rhodamine B in water and beverage samples by using spectrophotometer is very difficult because of low detection limit of instrument and matrix component of samples. In order to solve these problems separation and preconcentration procedures are necessary [2].

Switchable solvents recently used as an alternative green medium for different chemical and separation process [3]. Switchable hydrophilicity solvent (N,N-Dimethyl cyclohexylamine) was dispersed in an aqueous medium by the effervescent reaction of CO₂-table of (sodium carbonate and citric acid) to enhanced the contact area between two medium, which radically improve the extraction capacity of the rhodamine B from aqueous medium to switchable solvent. The phase separation was achieved by simple heating not by centrifugation that make a change on hydrophilicity to hydrophobicity. A new, simple and green switchable solvent extraction method was developed in this study. Various analytical parameters such as pH, volume of switchable solvent, etc. were optimized. A Pareto chart of standardized effect was applied to screening out through analysis factorial design in experimental studies. Matrix effects of concomitant ions were also studied. Limit of detection (LOD) and enhancement factor (EF) were achieved to be 0.045 µg L⁻¹ and 50, respectively. The accuracy of the present method was verified by analysis of real samples by spiking addition method. The relative standard deviation (RSD) was obtained 3.2%. The present method was applied to water, food and soft drink samples by using spectrophotometer.

Keywords: Rhodamine B; CO₂-table; N,N-Dimethyl cyclohexylamine; Switchable solvent; Spectrophotometer.

[1] M. Soylak, Y.E. Unsal, E. Yilmaz, M. Tuzen, *Food and Chemical Toxicology*, 49 (8), 2011, 1796-1799.

[2] N. Ozkantar, M. Soylak, M. Tuzen, *Turkish Journal of Chemistry*, 41 (6), 2017, 987-994.

[3] S.M. Mercer, T. Robert, D.V. Dixon, C.S. Chen, Z. Ghoshouni, J.R. Harjani, P.G. Jessop, *Green Chemistry*, 14(3), 2012, 832-839.

O-12

Neutron Measurements for Ferro Boron Alloys and Experimental Determination of Radiation Properties

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In the experimental study, the neutron capture properties of iron boron alloys containing different ratios of boron were investigated using ²⁴¹Am–Be neutron source and the Canberra NP-100B neutron detector. Transmission measurements were taken for alloys Fe99–B1, Fe98–B2, Fe96–B4, Fe94–B6, Fe92–B8, Fe90–B10, Fe88–B12, Fe86–B14, Fe84–B16, Fe82–B18, and Fe80–B20. Ferro - boron (Fe - B) is a binary alloy of iron with boron content between 10 % and 20 % and is the lowest cost boron additive for steel and other ferrous metals [1]. Iron is an important shielding material with a high atomic number that slow down fast neutrons with energies below 1 MeV [2]. It is possible to absorb the slowing neutrons with boron having a high absorption cross-section. Therefore, Ferro-boron is an alloy suitable for both to slow down fast neutrons and to absorb the slowing neutrons. The measurement results showed that as the boron ratio in the alloy increased, the number of neutrons reaching the detector decreased.

Keywords: Ferro - boron; Neutrons; Neutron shields.

Acknowledgements

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[1] Sahin, S., Meric, C., Saritas, S., *Advanced Powder Technology*, 21, 2010, 483– 487.

[2] D. Sarıyer, R. Küçer, N. Küçer. *Social and Behavioral Sciences*, 195, 2015, 1752 – 1756.

O-13

Evidence of Maskelynite Formation and Low Weathering of Didim Meteorite by Infrared and EDXRF Spectroscopy

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Didim meteorite (DM) that fell in Aydin, Turkey in 2007 is an ordinary chondrite and has been classified as H3–5. It was reported that chondrules and clasts in DM contain almost pure forsterite and enstatite compositions [1]. The aims of this study are to further identify chemical and molecular characteristics, investigate the maskelynite formation and determine the weathering profile of DM by Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) and EDXRF (Electron Dispersive X-Ray Fluorescence) spectroscopic techniques. ATR-FTIR spectrum of DM was collected on a Perkin-Elmer Spectrometer. XRF spectrum was collected on Rigaku NEXCG (Rigaku GmbH) XRF system and compositional and elemental data were obtained. Characteristic enstatite signatures were observed at 639, 687 and 725 cm⁻¹ as broad and low intensity peaks which is an indication of feldspar being transient state toward the maskelynite formation [2]. Si–O deformation of pyroxenes were observed at 639, 665 and 673 cm⁻¹, respectively [3]. Si–O asymmetrical vibration of enstatite was also confirmed from the bands at 880, 915 and 1122 cm⁻¹. Besides, two bands observed at 971 and 1000 cm⁻¹ are due to asymmetric stretching of olivine [2, 4, 5, 6]. According to XRF data based on Ba and Sr enrichment scheme, less altered meteorites have low concentrations of 4 and 10.2 ppm of Ba and Sr, respectively [7]. According to a previous report of compositions on DM from 2008, Ba and Sr compositions are 20.3 and 10.1 ppm, respectively [8]. Our XRF results performed in 2019 showed that Sr composition is 12 ppm. From these results, we could speculate that DM is a less altered meteorite after 12 years.

Keywords: Didim meteorite; IR spectroscopy; XRF spectroscopy; Weathering; Maskelynite.

[1] The Meteoritical Bulletin. 2008. 94:1570–1571.

[2] Gyollai I., Krebsz M., Kereszturi A., Berczi Sz., and Gucsik A. 2014. FTIR–ATR Spectroscopy of shock vein in Mócs L6 chondrite. Workshop on the Modern Analytical Methods Applied to Earth and Planetary Sciences. Proceedings of the Workshop on the modern analytical methods applied to Earth and Planetary Sciences, Sopron, Hungary, Nov. 1, 27–36.

[3] Jovanovski G., Makreski P., Kaitner B., Boev B. 2009. Croatica Chemica Acta 82:363–386.

[4] Saikia Bhaskar J., Parthasarathy G., and Sarmah N. C. 2018. Open Access Journal of Mathematical and Theoretical Physics 1:225–230.

[5] Jäger, C., F. J. Molster, J. Dorschner, T. Henning, H. Mutschke, and L. B. F. M. Waters. 1998. Astronomy and Astrophysics 339:904–916.

[6] Oehler H., and Günthard H. 1969. Journal of Chemical Physics 51:4719–4728.

[7] Al-Kathiri A., Hofmann B., Jull A. J. T., and Gnos E. 2005. Meteoritics & Planetary Science 40:1215–1239.

[8] Ozel M. E., Kocahan O., Sengul E. 2008. Türkiye'nin meteorit çarpma kraterleri envanteri: Kraterlerin morfolojik özellikleri ve uydu görüntüleriyle bulunması. (Unpublished TUBITAK project results: Project no:104T327).

O-14

**Theoretical Studies and Spectroscopic FT-IR and NMR Comparisons
of Two Pd-based N-heterocyclic carbene Complexes**

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This study contains spectroscopic and theoretical investigations of two N-heterocyclic carbene (NHC)PdX₂(morpholine) complexes. NHCs were used for years in the synthesis of important transition metal–NHC complexes in organometallic chemistry thanks to the unique ligand properties of the NHC precursors such electronic and steric adjustability, σ -donor and π -acceptor abilities. In this presentation, comprehensive theoretical calculations including the optimized structural parameters, the HOMO–LUMO energy gap, vibrational frequencies, chemical shifts were calculated by using density functional theory (DFT) with the B3LYP/LanL2DZ//6–31G* level and compared with the experimental data. FMO amplitudes and MEP diagrams were used to show the chemical activity of the complexes. In addition, natural bond analysis (NBO) was carried out to get detailed insight about the intra and inter-molecular bonding and interaction between bonds and to investigate charge transfer, delocalization or hyperconjugative interactions in the crystal structures.

Keywords: N-Heterocyclic carbene complex; Morpholine; FT-IR and NMR; DFT calculations.

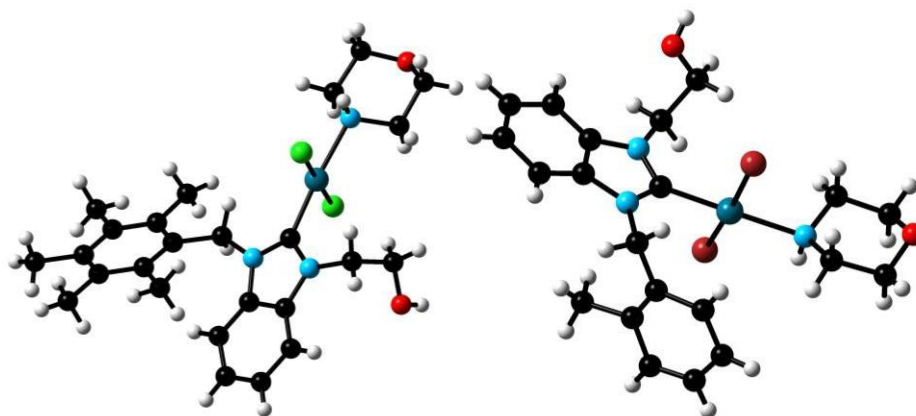


Figure 1. Optimized structures of the complexes with the B3LYP/LanL2dz//6–31G*.

O-15

Open Shell Ions Mobility In Cooled Helium Gas At 4.3K: Shallow Minimum Appearance

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This work is aimed to show the effect of the spin-orbit and the quantum-mechanical calculations on the behavior of the open shell C⁺ and N⁺ and O⁺ ions mobility in a cooled helium gas at the temperature of 4.3K. The experimental measurements of Tanuma and his team at Tokyo Metropolitan University using a mass-selected-ion-injected drift tube, of these ionic open shell systems, show usually the shallow minimum in the mobility at weaker electric field [1,2].

As to reveal theoretically this behavior of ionic open shell mobility, we calculated the ion-atom interaction potentials, including spin-orbit coupling, using high-level ab initio calculations [3]. Then, the quantal transport cross sections, needed in the computation of the mobility coefficients with Viehland gram-char Fortran code, are calculated in terms of the collisional energy of the the C⁺-He, N⁺-He, and O⁺-He systems. The Obtained results, at temperature 4.3K, show the spin-orbit interactions have the negligible effects on the mobility coefficients.

Keywords: Spin-orbit effects; Quantal cross sections; Ion mobility.

[1] S. Matoba, H. Tanuma and K. Ohtsuki, J. Phys. B At. Mol. Opt. Phys. 41 (14), 145205 (2008).

[2] J. Sanderson, H. Tanuma, N. Kobayashi and Y. Kaneko, J. Chem. Phys. 103 (7098) (1995).

[3] H.-J. Werner, P.J. Knowles, R. Lindh, F.R. Manby, M. Schütz, P. Celani, T. Korona, G. Rauhut, R.D. Amos, A. Bernhardsson, A. Berning, D.L. Cooper, M.J.O. Deegan, A.J. Dobbyn, F. Eckert, C. Hampel, G. Hetzer, A.W. Lloyd, S.J. McNicholas, W. Meyer, M.E. Mura, A. Nicklass, P. Palmieri, R. Pitzer, U. Schumann, H. Stoll, A.J. Stone, R. Tarroni, and T. Thorsteinsson, molpro, version 2002.6, a package of ab initio programs.

O-16

DFT and-[¹H, ³¹P, ¹¹⁹Sn]-NMR Investigation of the Cis-Trans Isomerization Mechanism of the Adduct SnCl₄.2HMPA* Complex

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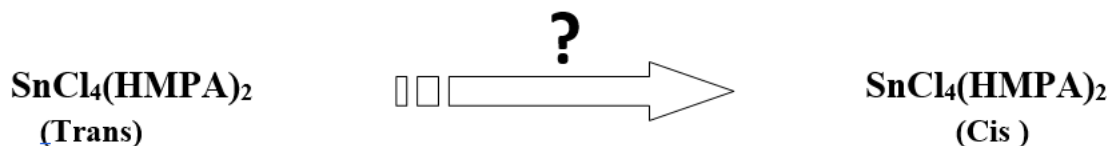
²Laboratoire de Spectroscopie Atomique Moléculaire et Applications, Faculté des Sciences de Tunis- Université de Tunis El Manar-Tunis TUNISIA

Using DRX [¹H] and [³¹P, ¹¹⁹Sn] MAS- NMR techniques, the SnCl₄.2HMPA complex in solid state has been shown to be all trans isomer. However, in solution both isomers cis and trans coexist in a dynamic equilibrium [2] and their relative ratio depends on the solvent polarity.

According to the importance of the reactivity of the cis and trans SnCl₄.2HMPA complex isomers in either catalysis or in microbiology domains, it appears to be a very interesting task to investigate the cis-trans isomerization mechanism. This could able us to get more insight about the previous experimental results and also to discuss the correlation between the SnCl₄.2HMPA catalytic activity and the cis-trans relative stability.

A very helpful way to characterize the cis-trans isomerization mechanism corresponds to a theoretical approach using DFT method implemented in Gaussian 09 program[3] combined to the 6-31G(d,p) basis set [4]. Our results show that the cis-trans isomerization is a rotating mechanism involving two Cl atoms and one ligand.

Keywords: Complex; NMR; Isomerism; Transition state; DFT.



*HMPA : ((CH₃)₂N)₃P=O

[1] L.A. Aslanov, V.M. Ionov, V.M. Attiya, A.B. Permin, V.S. Petrosyan, Zhur. Strukt. Kim. 18 (1977) 1103

[2] M.T. Ben Dhia, M.A.M.K. Sanhoury, L.C. Owono Owono, M.R. Khaddar, J. molec. Struc. 892 (2008) 103

[3] Gaussian 09 program.

[4] V. Rassolov, M.A. Ratner, J.A Pople, P.C. Redfern, L.A Curtiss, J. Comp. Chem.,22 (2001). 976

O-17

Short-Lived Intermediates in Photochemistry of p-Arsanilic Acid: A Laser Flash Photolysis Study

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p-arsanilic acid (p-ASA) is a representative of phenylarsonic feed additives have been used widely in the livestock and poultry industries as antibiotics for promoting the growth of animals. The large usage, good water solubility and slow biotransformation of these organic arsenic additives lead to their release into in groundwater and surface waters. Though phenylarsonic feed additives themselves possess the low toxicity their biological and (photo)chemical transformation can lead to the generation of toxic inorganic arsenic and other organic by-products. Because of this it is necessary to understand photochemical degradation pathways of this compound during solar irradiation in natural water systems [1, 2] or during UVC disinfection treatment applied to farm wastewater [3, 4].

In this talk we present new insight in mechanism of p-ASA photochemistry which was reinvestigated for the first time by means of laser flash photolysis ($\lambda = 266 \text{ nm}$) coupled with high resolution LC-MS. Main primary photoprocess was found to be a monophotonic ionization ($\phi^{266\text{nm}} = 0.032$) leading to formation of hydrated electron and corresponding aniliny radical. These primary species react with dissolved oxygen with formation of reactive oxygen species and peroxy radical. These secondary species are responsible for formation of main organic photoproducts such as aminophenol and different dimeric products. Dependence of quantum yield of p-ASA photodegradation upon excitation wavelength was obtained for the first time. It was found that its value is slowly drops in the region 222 – 308 nm from 0.058 to 0.035. These findings seem to be crucial to understand a fate of p-ASA during UVC disinfection or sunlight photolysis.

Keywords: p-arsanilic acid; Primary processes; Photodegradation; Laser flash photolysis.

Acknowledgements

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[1] X. Zhu, Y. Wang and C. Liu, Chemosphere, 2014, 107, 274-281.

[2] X. Xie, Y. Hu and H. Cheng, Wat. Res., 2016, 96, 136-47.

[3] S. Li, J. Xu, W. Chen, Y. Yu, Z. Liu, J. Li, F. Wu, J. Environ. Sci. 2016, 47, 39-48.

[4] J. Xu, X. Shen, D. Wang, C. Zhao, Z. Liu, I.P. Pozdnyakov, F. Wu, J. Xi, Chem. Eng. J., 2018, 336, 334.

O-18

Phenolic Profiling of *Allium scorodoprasum* subsp. *rotundum* by LC-MS/MS and Evaluation of Its Biological Activity

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Several species of *Allium* genus, particularly cultivated forms, namely *Allium sativum* (garlic), *Allium cepa* (onion) and *Allium porrum* (leek) are widely used in the human diet as spices and vegetables. *Allium scorodoprasum* subsp. *rotundum* known by the common name “wild leek”, or “wide garlic” is the ingredient of a traditional cheese of Turkey also the plant’s onion and leaves are consumed raw or cooked [1]. The aims of this study were to define the phenolic profile and enzyme inhibitory activities of bulb, stem and flower extracts of *A. scorodoprasum* subsp. *rotundum* collected from Kemalpaşa, İzmir. The presence and content of 30 selected phenolic compounds in methanol extracts of samples were investigated by LC-MS/MS, where 28 compounds were quantified, most abundant being: 3-hydroxybenzoic acid, 4-hydroxybenzoic acid, *p*-coumaric acid and 2 compounds were determined in trace amounts. And also, acetylcholinesterase, butyrylcholinesterase and tyrosinase inhibitory activities of samples were assessed spectrophotometrically by using a micro-plate assay modified from Ellman’s method and Masuda’s method with 96-well micro-plate reader [2, 3]. The extract of flower parts was found to exhibit significant activity respectively (IC₅₀ = 34.25, IC₅₀ = 9.32, IC₅₀ = 97.11 µg/ml).

Keywords: LC-MS/MS; *Allium*; Enzyme Inhibitory Activity.



Figure 1. *Allium scorodoprasum* subsp. *rotundum*.

Acknowledgements

This study was financially supported by TUBITAK (217S341).

[1] Mehmet Firat, Manas Journal of Agriculture and Life Science, 5 (1), 2015, 80–86.

[2] George L. Ellman, K. Diane Courtney, Valentino Andres Jr., Robert M. Featherstone, Biochemical Pharmacology, 7, 1961, 88–95.

[3] Toshiya Masuda, Daiki Yamashita, Yoshio Takeda, Shigetomo Yonemori, Bioscience, Biotechnology, and Biochemistry, 69 (1), 2005, 197-201.

O-19

Studies of Imprinting Conditions and Recognition Performance of Pirimicarb-Imprinted Sensor Chip

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This study describes the preparation of pirimicarb imprinted poly(ethyleneglycol dimethacrylate)-N-methacryloyl-(L)-tryptophan methyl ester based a new surface plasmon resonance (SPR) sensor for pirimicarb determination. SPR sensor chip using molecularly imprinted polymer (MIP) as sensing material has been developed for fast and onsite determination of pirimicarb in contaminated vegetables. Poly(ethyleneglycol dimethacrylate)-N-methacryloyl-(L)-tryptophan methyl ester based film on chip surface was synthesized by ultra violet (UV) polymerization for the detection of pirimicarb at low concentrations. At the first step, N-methacryloyl-(L)-tryptophan methyl ester complex was formed with pirimicarb and then, the pirimicarb imprinted nanofilm has been prepared. The characterization of the polymeric nanofilm has been conducted with ellipsometry, contact angle, fourier transform infrared-attenuated total reflectance and atomic force microscopy measurements. The repeatability of pirimicarb imprinted chip was investigated by using of equilibration-binding-regeneration cycles for five times. The sensor chip developed exhibits good selectivity (low response to those pesticides with similar structures to pirimicarb, such as atrazine and propoxur), high sensitivity to pirimicarb with a linear working range from 0.04 to 4.20 nM and a detection limit (S/N = 3, n = 5) of 0.031 nM. According to the results, the present proposed technique is a promising tool for the preparation of the receptors which could recognize pirimicarb pesticide in contaminated vegetables. Also, the SPR sensor chip has showed low-detection limit, high selectivity and sensitivity for pirimicarb assay.

Keywords: Molecularly imprinted polymer; Pirimicarb; Sensor; Chip.

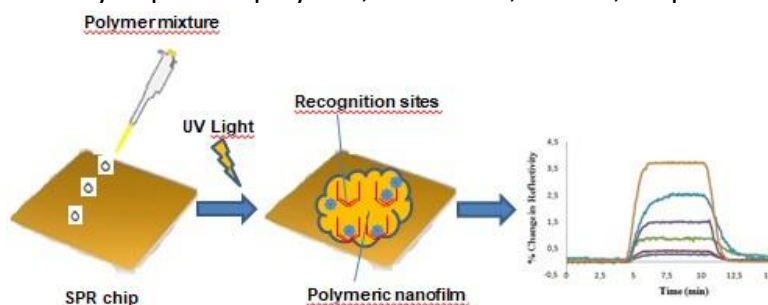


Figure 1. Schematic representation of pirimicarb imprinted SPR sensor chip surface.

Acknowledgements

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O-20

A Review of Studies on Monitoring Self-Healing Processes by the Help of Different Types of Spectroscopy

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Studies on self-healing materials are rapidly increasing and many new projects are arising with the development of technology. These materials provide great convenience in many areas of the industry. While self-healing concrete plays a game-changing role in the field of construction, self-healing polymer materials provide many advantages in defense and electronics industries. Chemically and physically investigation of the self healing processes is really an important issue to be concerned due to difficulties faced with during analyzes and tests. Thus, there are many new researches addressed to work on techniques to facilitate understanding of these processes recently. Spectroscopy is a highly preferred technique due to fact that it provides a non-destructive examination. In this study, studies performed in this area have been analyzed and summarized. In addition to literature review, it was benefited from various sources. As a result, it has been concluded that different types of spectroscopic techniques provide advantages over different materials. While broadband dielectric spectroscopy (BDS) mainly provides significant contributions to elastomers, usage of raman spectroscopy makes contributions to polymers and biopolymers due to high spatial resolution. As far as self-healing concrete concerned, then Scanning Electron Microscopy Test (SEM) and Energy-Dispersive X-ray Spectrum (EDM) are mainly used to understand the healing processes. In the future, it is expected that many other techniques will be used thanks to new promising studies.

Keywords: Spectroscopy; Self-healing materials; Broadband Dielectric Spectroscopy; Self Healing Concrete; Raman Spectroscopy.

O-21

Investigation of the Properties of a Magnetically Modified High Aspect Ratio Chestnut Shell Nanobiosorbent Using Mössbauer Spectroscopy and FTIR

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Magnetically modified nanobiomaterials are functional due to their response to external magnetic field. This important feature can be used to address the problem of water pollution caused by textile dyes which are known to have potential toxic and carcinogenic effects on human. For this purpose, biosorption technique has advantages like low cost, effectiveness, high efficiency and environmental friendliness over other techniques used. The production of a nanobiosorbent with magnetic properties and high specific surface area with a mesoporous structure is beneficial not only for experimental purposes but also for industrial scale applications. The magnetic properties that nanobio-composite possess are useful for the removal of dyes from waste water as they can easily be eliminated from the solution after the treatment. Here in this study, chestnut shell was magnetically modified with magnetite to produce a new nanobiosorbent and its magnetic properties were examined using Mössbauer spectroscopy. In addition, FTIR, BET and SEM were used for material characterization. The Mössbauer spectra for the sample are consisting of two magnetic zeeman sextets and one paramagnetic doublet. According to the parameters of Mössbauer Spectra, the material has a crystal structure with cubic symmetry. The data collected from FTIR confirms the presence of Fe₃O₄ nanoparticles according to the peak observed around 466 cm⁻¹. This new nanobiomaterial could also be used as a carrier for immobilization of bioactive compounds and potential biotechnology applications.

Keywords: Mössbauer spectroscopy; FTIR; Magnetic; Nanobiosorbent; Chestnutshell.

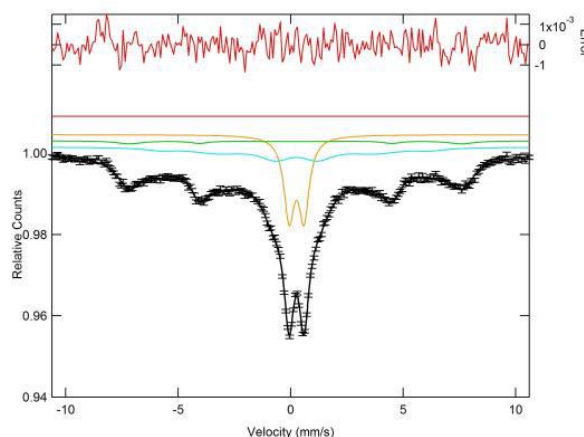


Figure 1. Mössbauer spectrum of magnetically modified chestnutshell nanobiosorbent.

Acknowledgements

The authors gratefully acknowledge Dr. Hakan GÜNGÜNEŞ for fitting the Mössbauer spectrum and his helpful discussion regarding this data.

- [1] Meng, Fanqing, et al. "Novel dendrimerlike magnetic biosorbent based on modified orange peel waste: adsorption–reduction behavior of arsenic." *ACS Sustainable Chemistry & Engineering* 5.11 (2017): 9692-9700.
- [2] Lujanienė, G., et al. "Magnetic graphene oxide based nano-composites for removal of radionuclides and metals from contaminated solutions." *Journal of environmental radioactivity*, 66 (2017): 166-174.

O-22

A Biophysical Study of the Interactions Between Citrus Flavonoid Hesperidin and Membrane Lipids

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Flavonoids are generally found in the plant kingdom indicating a diverse range of biological efficiencies, containing antibacterial, antifungal, antiviral, anti-allergic, anti-inflammatory, antiproliferative and antioxidant activities [1–4]. In order to understand the several useful effects of flavonoids on health, more studies associated with structural aspects of the flavonoid interaction with membrane systems have to be performed. In this study, we determined the mechanism of the interactions between citrus flavonoid hesperidin and model membrane lipids and the alterations were examined using Differential Scanning Calorimetry (DSC) and Fourier Transform Infrared (FTIR) Spectroscopy. We found that hesperidin causes changes in the arrangement of the polar heads of lipids, membrane dynamics and the main phase transition temperature of membrane lipids. Hesperidin-induced changes in model membranes may be generalized to biological membranes and may contribute to the practical use of this compound in prevention and treatment of diseases.

Keywords: Citrus flavonoid; Hesperidin; Membrane lipids; DSC; FTIR.

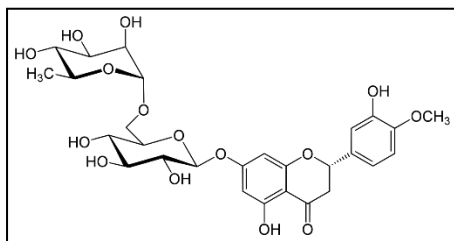


Figure 1. Chemical structure of hesperidin.

Acknowledgements

This work was supported by Ege University Scientific Research Projects Coordination Unit. Project Number: 18-FEN-030.

- [1] H. Cheong, S.Y. Ryu, M.H. Oak, S.H. Cheon, G.S. Yoo, K.M. Kim, Arch. Pharm. Res., 21, 1998, 478–480.
- [2] V. García-Mediavilla, I. Crespo, P.S. Collado, A. Esteller, S. Sánchez-Campos, M.J. Tuñón, J. González-Gallego, Eur. J. Pharmacol., 557, 2007, 221–229.
- [3] T.P.T. Cushnie, A.J. Lamb, Int. J. Antimicrob. Agents, 26, 2005, 343–356.
- [4] A.B. Hendrich, Acta Pharmacol. Sin., 27, 2006, 27–40.

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Poster Abstracts

P-01

New 5-arylidene-4-thiazolidinone, Synthesis, UV/Vis-Absorption and Fluorescence Spectroscopic

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4-Thiazolidinone has an important role as a widely exploited pharmacophore in medicinal chemistry having varied biological activity such as antifungal, antibacterial, anticancer, antioxidant, anti-inflammatory, COX-1 inhibitory etc. [1]. In addition, this nucleus appears in many fluorescent compounds that have useful applications such as fluorescent markers or as light emitters in organic light emitting devices (OLEDs) [2].

In this work, we report in figure 1, the synthesis of a new class of structurally novel 5-arylidene-4-thiazolidinone **5a-f** derivatives incorporating pyrone and 4-thiazolidinone nuclei. The reaction of thiosemicarbazones [3] **3a-c** with ethyl bromoacetate yielded the corresponding 4-thiazolidinones **5a-c**. The compounds **7a-f** were further reacted with aromatic aldehydes (benzaldehyde, methoxy benzaldehyde) in presence of few drops of pyridine and piperidine in dichloroéthane under reflux, resulting in the formation of single products **5 a-f** in moderate yield (39-55 %).

The synthesized products were characterized by IR, ¹H RMN and ¹³C RMN. The evaluation of UV/vis and fluorescence properties of these compounds was carried out.

Keywords: 3-halogenothiophene-2-carbaldehyde; DFT; Vibrational spectra; Halogen effect.

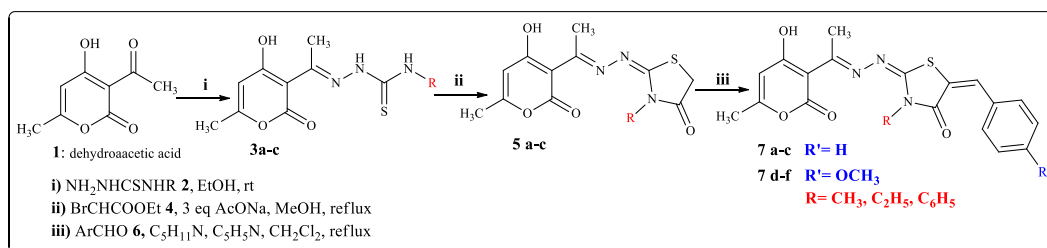


Figure 1. Synthetic pathway to generate 5-arylidene-4-thiazolidinone **7 a-f**.

[1] Chate, A. V.; Tathe, A. G.; Nagtilak, P. J.; Sangl, S. M.; Gill, C. H, *Chinese J Catal*, 37 (11), 2016, 1997-2002.

[2] Costa, S. P. G.; Batista, R. M. F.; Sousa, A. M. R. C.; Raposo, M. M. M. *Mater. Sci. forum*, 514-516, 2006, 147-151.

[3] Nechak, R.; Bouzroua-Aichouche, S.; Benmalek, Y.; Salhi, L.; Poulain-Martini, S.; Morizur, V.; Dunach, E.; Nedjar- Kolli, B, *Synth. Commun*, 45 (2), 2015, 262-72.

P-02

An Efficient and Catalytic One-Pot Coupling Method for the Synthesis of Novel Pyran and Furan Derivatives

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Pyran derivatives are found in various natural products. They gained considerable attention due to their wide spectrum of biological activities such as antibacterial, antitumor agents and HIV protease inhibitors [1]. Also, many furan-ring structures were evaluated for their applications in pharmacology and medicinal chemistry such as antidepressant, anxiolytic and anti-inflammatory agents [2]. The several synthetic strategies developed in the literature used the protic catalysis to generate pyran and furan heterocycles.

The aim of this work is to develop an easy, new green method, based on a not polluting and not toxic catalysis, in one-process for the synthesis of this class of compounds, starting from pyrone and allylic acetate derivatives, using metal triflates (M(OTf)_n) as the catalyst.

In Figure 1, we describe an example of the condensation of 4-hydroxycoumarin **1a** with prenyl acetate **2a**, under metal triflate catalysis, to give a mixture of 3,3-dimethyl-3,4-dihydropyrano[3,2-b]chromen-10(2H)-one **3aa** and 2,2-dimethyl-3,4-dihydropyrano[3,2-c]chromen-5-(2H)-one **4aa**, in 86 % yield in a ratio of 77/23. The protocol was extrapolated to the synthesis of various pyranofuran, pyranopyrone and furanopyran derivatives. Moreover, we report some rearrangement studies of linear pyranochromone **3aa** to angular pyranocoumarin **4aa**.

Keywords: Coumarine; Triflates; Cyclization; Pyran; Furan.

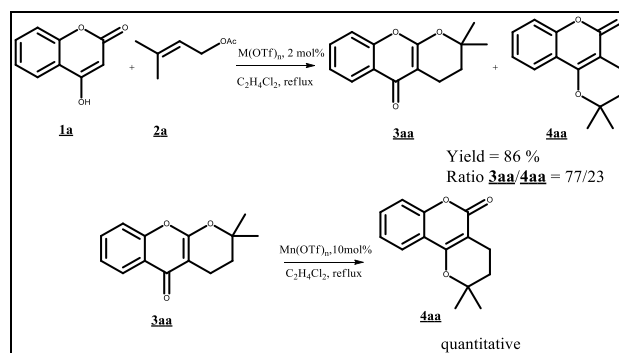


Figure 1. Synthesis of linear pyranochromone **3aa** and angular pyranocoumarin **4aa**.

[1] Sari, E., Aslan, H., Dadi, S., Oktemer, A., Logoglu, E. GU J Sci, 30 (4), 49-55, (2017).

[2] Katircioğlu, H., Loğoğlu, E., Tilki, T., Öktemer, A. Med. Chem. Res, 16 (5), 205-212, (2007).

P-03

Spectroscopic Identification of Pigments used in Icons from the Church St. George, Struga

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The study is focused on the use of several elemental analytical methods for the analysis of painted works of art including: X-ray fluorescence (XRF) performed in the National Conservation Centre-Skopje, particle induced X-ray analysis (PIXE) carry out in the Laboratory of Ion Beam Applications, Debrecen, Hungary and scanning electron microscopy (SEM) made in the Diagnostic Science Laboratories, Kalkara, Malta. The measurements were taken on the cross-sections and paint fragments to characterize pigments and provide additional information complementary to existing investigations such as optical microscopy and classical chemical analyses.

These techniques are the most widely used in the field of cultural heritage, providing the elemental composition of materials in a non-invasive and non-destructive way. This paper reports the analysis of the pigments and ground layers on a traditional wooden paintings-icons belonging to different centuries from the church St.George located in the western part of North Macedonia. Selected icons presented in this paper belong to different periods made by various painters from the district of Struga. The subject of analysis was a medieval 13th century icon, two double painted icons from the 16th-20th century and two icons from the 18th century, distinguished by their author and specific painting technique.

Combined diagnostic investigations aim in achieving a better preservation and conservation of our cultural heritage by increasing the knowledge of art objects through advanced chemical and physical analyses. Conservation is often assist by analytical techniques that offer rapid materials identification with minimal intervention or side effects on the object being examine. The pigments used in these objects, are characteristic for the period in which the art object was made, their provenance and, in a most of the cases, the individual artist.

Keywords: Spectroscopic analyses; Identification; Pigments; Icons.

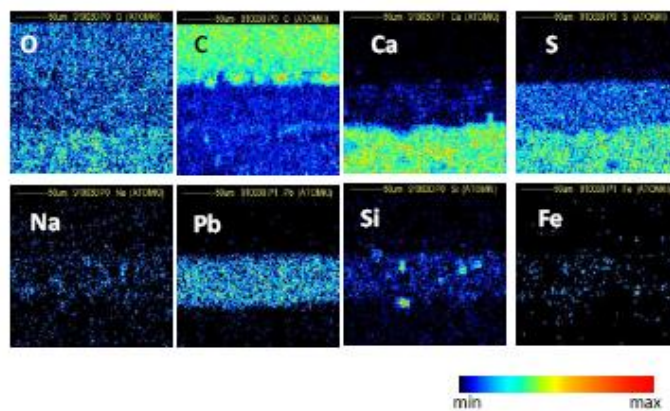


Figure 1. Elemental maps and measurement on the identified pigment layers with PIXE, sample 1r3j.



Figure 2. Sampling scheme of Icon St. George (1266/7) in Struga, areas analyzed by XRF, PIXE and sample site for paint-cross section are marked on the image.

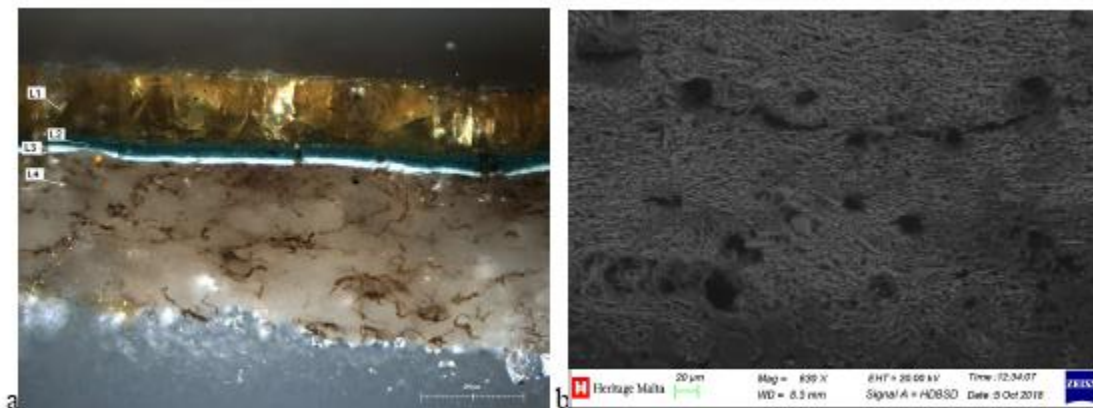


Figure 3. a) Microphotography of cross section from green pigment applied over the white ground b) SEM image of the same sample.

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[1] Angelina Popovska, Svetlana Mamucevska-Miljkovikj, Conservation investigations and XRF analysis of the icons of St. George from Struga (1266-67), Saopštenja, XLVI, 2014, 313-324.

[2] P.Miljkovic –Pepek, L'icōne saint Georges de Struga, oeuvre du peintre jean, Cah. Arch XIX, Paris,1969, 213-221.

[3] Gergő Bétéri, Zsófia Kertész, Enikő Papp, Zita Szikszai, Zoltán Szoboszlai, ZsófiaTörök (Atomki IBA Laboratory), IPERION-CH TNA Project IOPL, Investigation of the Structural Layers of the Icon St.George from Struga Dated from 1267 year, 2017.

[4] V. Popovska - Korobar, Ohrid-Struga iconographic traces from the second half of XV century, Patrimonium, Skopje, 2010, 289-299.

[5] R. Ljubinkovic-M. Chorović, Medieval painting in Ohrid, Symposium, Ohrid, 1961, 113.

P-04

The Role of the Nanoparticles Systems with Vitamins B on the Stratum Corneum

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Vitamins are essential for human health. Positive effect of vitamins remains unclear in terms of local application for wound healing. Certain combinations of B vitamins demonstrate a positive influence on human keratinocytes and fibroblasts. Vitamins promoted fibroblast migration, and a statistically significant induction of keratinocyte proliferation was observed. Therefore, local vitamin application could benefit the physiologic wound healing process [1]. Nevertheless, most topically applied drugs without penetration enhancers will not achieve active skin penetration [2, 3]. Various nanoparticles (NPs) are used to accelerate the penetration of medicaments through the skin, for the targeted drug delivery or in the case of surgical implants. Moreover, NPs play an important role in cosmetics. The development of biocompatible/environmentally friendly NPs is necessary. One of the possible penetration enhancers are silver NPs (AgNPs) [2]. The aim of this study was to evaluate the penetration of riboflavin, pantothenic acid and panthenol with varying diameters of AgNPs (20 nm, 40 nm, 60 nm and 100 nm) as penetration enhancers. Each B vitamin/vitamin derivative was dissolved in AgNPs hydrosol to the concentration $c = 0.001$ mol/L and stored in the refrigerator for 24 hours to adsorb the analyte on the surface of AgNPs. Subsequently, the samples of pig skin were treated with the B vitamin-NPs system. Attenuated Total Reflection (ATR) technique of infrared spectroscopy was used for investigation of the interactions in the uppermost layer of the *stratum corneum* (ca. 2 μm); for the depth profile measurements (tens of μm), confocal Raman microscopy was used. The samples of pig skin were treated by AgNPs hydrosols with B vitamins/vitamin derivative for 4 hours. Hundreds of vibrational spectra of the treated skin samples were evaluated by multivariate statistical methods, namely Principal Component Analysis (PCA) and Soft Independent Modelling of Class Analysis (SIMCA) for classification and Partial Least Squares (PLS) for examination of B vitamins/vitamin derivative time dependent effect on the skin. From Raman depth profile spectra of the treated skin samples we got information about distribution of B vitamins/vitamin derivative in the skin layers. The diameters of AgNPs strongly influence the penetration properties of the *stratum corneum* layer.

Keywords: Stratum corneum; B Vitamins/Vitamin derivative; Silver nanoparticles; Vibrational spectroscopy; Multivariate statistical methods.

Acknowledgements

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- [1] Julian-Dario Rembe, Carolin Fromm-Dornieden, Ewa Klara Stuermer, *Advances in Skin & Wound Care*, 31, 5, 2018, 225-233.
- [2] Adéla Jenišťová, Marcela Dendisová, Pavel Matějka, *European Journal of Pharmaceutics and Biopharmaceutics*, 116, 2017, 85-93.
- [3] Adéla Jenišťová, Laura Halajová, Marcela Dendisová, Pavel Matějka, *Vibrational Spectroscopy*, 97, 2018, 119-128.

P-05

Label-Free Bacteria Detection and Discrimination using Raman and Ultrasensitive Surface-enhanced Raman Spectroscopy

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The need of rapid detection methods with high sensitivity and specificity for bacterial identification is at high demand in today's society. Among the spectroscopic techniques used for bacteria identification, Raman spectroscopy is a real-time detection method with the ability to quickly and effectively detect a variety of chemical structures and material composition, with more specific and readable biological or chemical information than the infrared spectroscopy [1]. A very powerful technique with an increasing popularity is surface enhanced Raman scattering (SERS) spectroscopy. It relies on the interaction between the target analyte and SERS-active metallic nanostructures, permitting single bacterial cells identification. Here we demonstrate the successful detection and discrimination of two relevant Gram-positive bacteria species, *Lactobacillus casei* (*L. casei*) and *Listeria monocytogenes* (*L. monocytogenes*) using Raman and SERS spectroscopies, coupled with principal component analysis (PCA) [2]. *L. casei* and *L. monocytogenes* are Gram-positive, rod shaped, anaerobic bacteria. The Raman spectra of *L. casei* and *L. monocytogenes* showed very similar bands, in terms of band position and intensity. The detected Raman bands arose mainly from adenine and purine-like molecules, proteins (amide bands), but also from the unsaturated lipids from the peptidoglycan layer. The existing differences between the two investigated bacteria were only noticeable when PCA was applied on the Raman results and they were fairly discriminated. In case of the SERS results, two synthesis methods of the silver (Ag) SERS-active nanomaterials were used and the recorded spectra were analyzed. The two different SERS substrate synthesis protocols provided similar and reliable information that enabled bacterial differentiation using PCA analysis by explaining around 30% of the total variance.

Keywords: SERS; Raman; Gram-positive bacteria; Label-free detection; PCA.

Acknowledgements

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- [1] Xihong Zhao, Mei Li, Zhenbo Xu, *Frontiers in Microbiology*, 9, 2018, 1236.
- [2] Alia Colnita, Nicoleta Elena Dina, Nicolae Leopold, Dan Cristian Vodnar, Diana Bogdan, Sebastian Alin Porav, Leontin David, *Nanomaterials*, 7, 2017, 248.

P-06

Polymethylsilsesquioxane Concentration Effects on the Nanostructures and the Biophysical Properties of some Foundations and BB Creams

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Liquid foundations and BB creams are widely used in cosmetic industry to make the face appear slimmer. R&D studies are also increased to reach more fresh and hydrating texture and firms the beautiful skin for a more youthful effect. The nano scale formations may be quickly effected by the slightly changed polymer ratios and very effective on the biophysical and biochemical properties of these cosmetic products, even though the molecular components of the formulations are not very different. NSRRC, BL23A endstation was used for experimental studies to obtain nanoscale structural changes by using SAXS and WAXS methods. It was shown that polymer concentrations of Polymethylsilsesquioxane which is widely used in cosmetic products such as foundations and BB creams are very effective on nano aggregations and the products' properties. 3D shapes of the nanoaggregations deviate from globular form (POSS) to the more crystalline layered (OC) fractal forms [1] with the increased polymer concentration as seen in Fig.1. Beside of the shape, the sizes (Radius of Gyration values: Rg) of the nanoglobules are also changing in the range of 23.6-33.0 nm. UV protection (absorption, reflection and transmission) properties, molecular scale structural changes (obtained with FT-IR spectroscopic analyzes) and anti-biofilm activities were also carried out and investigated according to the different polymer concentrations.

Keywords: Cosmetic creams; PMSQ; Nanoscopic analyses; SAXS; UV; FT-IR; Bioactivity.

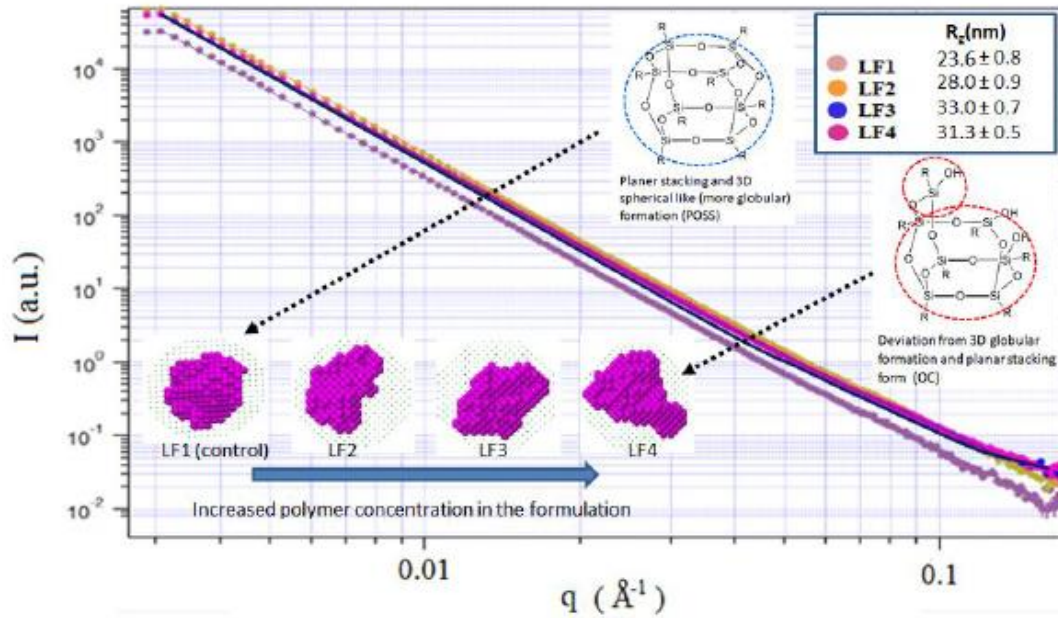


Figure 1. Graphical representation of the fitted Small Angle X-ray Scattering Data ($I(q)-q$), the obtained nano structural results (the sizes and 3D morphologies) and the most possible fractal unit contents (POSS and OC) related with liquid foundations according to the studied polymer concentrations.

Acknowledgements

The study was supported with FYL-2018-17456 coded Hacettepe Univ. BABK Project.

[1] Abdessamad Baatti et al., Advanced Powder Technology, 28, 2017, 1038–1046.

P-07

Contribution of Infrared Spectrophotometry in the Analysis of Urolithiasis

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In this study, Fourier Transform Infrared Spectrophotometry (FTIR) analysis is used to analyze urinary tract stones. These calculi often have a heterogeneous composition including on average 3 to 4 components that can be of multiple natures (mineral, organic etc.). FTIR spectrophotometry has the advantage of analyzing in addition to crystalline substances, non-crystalline components (amorphous, oily lipids and proteins) often present in these calculi. Thus, it provides to extract the necessary information of the qualitative and quantitative composition of the lithiasis elements in order to elucidate the processes of their lithogenesis and to establish adequate etiological orientations. This technique also has other advantages such as the ability to detect up to 7 different components per spectrum, to analyze very small quantities of samples with rapid spectral acquisition. However, the analysis of the FTIR spectra required a lot of experience and know-how, particularly in the case of a mixture of several components in the same calculi. In this work we will elucidate certain aspects in the analysis of FTIR spectra in the case of mixtures of oxalocalcic (Whewellite - Weddellite), oxalocalcic - phosphocalcic and finally oxalocalcic - purine components. The Figure 1 illustrates the evolution of the FTIR absorbance spectrum in the case of majority calculi in anhydrous uric acid (AU0) in the presence of uric acid dihydrate (AU2), ammonium urate and calcium oxalate monohydrate. (Whewellite)

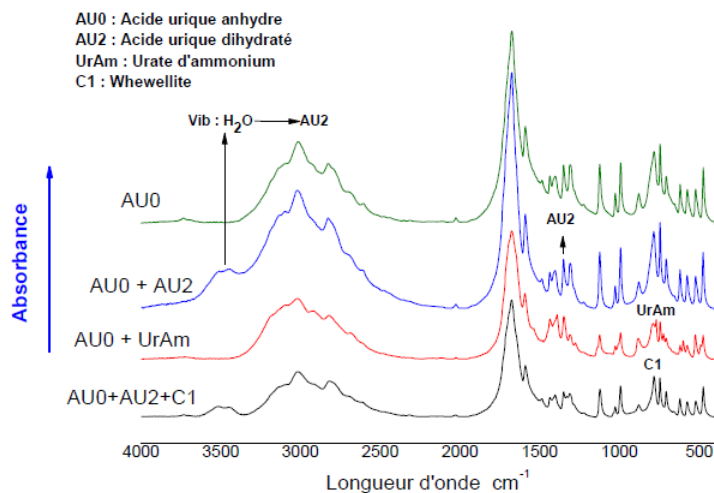


Figure 1. Example of similarities between purine IR spectra (AU0, AU2 and UrAm): Difficulty distinguishing C1 from AU2 in a majority calculat in AU0.

Keywords: Urolithiasis; Spectrophotometry IRTE; Weddellite; Purine.

[1] Leusmann CA, Macclure GL, Smolens I. Identification of renal calculi by computerized infrared spectroscopy. Clin Chim Acta 1988; 1733: 107-116

[2] Estepa L et Daudon M. Contribution of Fourier transform infrared spectroscopy to the identification of urinary stones and kidney crystal deposits. Biospectroscopy 1997;3(5):347-69.

[3] Basiri A, Taheri M, Taheri F. What is the state of the stone analysis techniques in urolithiasis? Urol J 2012;9(2):445-54.

P-08

2D Structures in Full-biobased Polyamide Nanocomposites Characterized by Raman Spectroscopy

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Graphene based nanocarbon [1] and other 2D non-graphene type materials have been reported as fillers for polymer nanocomposites with certain roles in physical properties (mechanical strength, thermal stability, etc.). Raman spectroscopy is a modern, effective and non-destructive method [2] used to assess the vibrational states of the groups in 2D structure molecules and can highlight the modifications occurred during the nanocomposites obtaining processes. This work aims to investigate and characterize innovative nanocomposites based on 2D structures and a full biobased polyamide 1010 (PA1010) - using Raman spectroscopy. Two types (C500 and M5) of graphene nanoplatelets (GNP) were used in different concentrations (for the graphene based 2D structures). For non-graphene type 2D structures, an eco-friendly layered double hydroxide (LDH) was chosen namely a hydrotalcite. A complete Raman assessment was performed on the nanocomposites obtained by extrusion, followed by injection moulding. The vibrational profile of the nanocomposites with 5% LDH was also examined. The positions, widths and intensities of the D, G and 2D peaks and additionally the relative intensity ratio ID/IG have been investigated. We observed an increase of the ID/IG ratio while the graphene concentration decreases, which suggested an increase of the defects in the graphene sp² planes. These aspects can be associated by a possible exfoliation of the graphene nanoplatelets in the polymer matrix (after processing) [3, 4].

Keywords: Raman; Bio polyamide; Nanocomposites; Graphene; Layered double hydroxides.

Acknowledgements

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[1] Jongwon Kima, Jinwoo Oha, Kyung Yeol Leec, Inhwa Jungb, Min Park, *Composites Part B*, 114, 2017, 445-456.

[2] Ming Xia, *International Journal of Spectroscopy*, 2018, 9 pages.

[3] Sergey V. Polschikov, Polina M. Nedorezova, Alla N. Klyamkina, Anton., Kovalchuk, Alexander N. Shchegolikhin, Vitaliy G. Shevchenko, Vyacheslav E. Muradyan *J. Appl. Polymer Sci*, 127, 2013, 904-911.

[4] J.Theo Klopogge, Ray L.Frost, *Journal of Solid State Chemistry*, 146, 1999, 506-515.

P-09

Influence on the Experimental Conditions on the SERS Signal of Nodularin Cyanotoxin

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Aquatic biotoxins detection using Raman spectroscopy techniques in relevant environment requires consolidated experimental data on the toxins molecular structure and their characteristic signature in various conditions, to include the experimental ones and the independent, environmental conditions. Additionally, co-existence of different related toxins species as well as their relationship with the algal-blooming events in environmental waters is a common challenge for developing new Raman-based sensing methods of toxins [1]. Along with microcystins, nodularins (NOD) are a class of cyanobacteria toxins occurring in environmental brackish waters [2]. Here, we investigate the influence of the laser energy, exposure time and collecting optics on the Raman and SERS spectra of nodularin, aiming to develop optimal sensing route via Raman techniques. We found that longer acquisitions time (20-600s) under low laser power better reproduced Raman of nodularin microcrystals obtained via drop-coating deposition technique [Brezestean et al, 2018][3] while SERS measurement in solution showed different feature from those obtained by drop coating deposition. The discussion of possible mechanisms involved in different SERS output is provided.

Keywords: Cyanotoxin; Nodularin; Drop coating Raman; SERS.

[1] S. Cintă Pinzaru ,Cs. Müller ,I. S. Tódor , B. Glamuzina, V. Chis, *Journal of Raman Spectroscopy*, 47,6, 2016, 636-642.

[2] Fewer, D.P., Jokela, J., Pauku, E., Österholm, J., Wahlsten, M., Permi, P., Aitio, O., Rouhiainen, L., Gomez-Saez, G.V., Sivonen, K., *PLoS One* 8, 9, 2013, 1–10.

[3] I. Brezestean, L. David, V. Chis, S.Cinta Pinzaru; 6th *International Biophysics Congress*, 2445-43111, S2, 85, 2018, Castellon, Spain.

P-10

The Effect of Methotrexate on Testis

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MTX is a folic acid antimetabolite; For the first time treating children's leukemias in 1948, the treatment of leukemia, lymphoma, osteosarcoma, lung cancer, breast cancer, bladder cancer, testicular tumor and foreign linguist belt therapy, as anticancer drug for many years, including psoriasis, dermatomyositis, sarcoidosis and rheumatoid In some cases, such as arthritis (RA), infectious diseases are also common. MTX is the 4-amino, N10-methyl analogue of folic acid in chemistry. Folic acid is the precursor of tetrahydrofolate which is important in DNA synthesis. Methotrexate inhibits tetrahydrofolate synthesis by tightly binding to and inhibiting the active site of the dihydrofolate reductase enzyme. This causes the synthesis of purine bases (adenine and guanine) required for DNA and RNA to stop. It also causes a breakdown of protein synthesis. In some studies, it is known that MTX-induced organ damage may be the result of oxidative stress. This oxidative stress causes damage to the structure of the testis and germ cells. After MTX administration, it has been reported that the decrease in sperm count, sperm DNA damage and seminiferous tubules in the testes, and permanent azoospermia and infertility in men were determined as side effects of chemotherapeutics. Antioxidant levels of cancer patients have been reported to be important in terms of chemotherapy efficacy. In patients treated with antioxidants, antioxidants are recommended to compensate for this loss. In studies related to chemotherapy and cancerous humans and animals, it is stated that sperm and testis tissue freezing processes, hormone applications, in vitro spermatogenesis can be done by testicular biopsy, testicular transplantation and antioxidant applications can prevent undesired effects on male reproductive system before and during chemotherapy. In the studies, it has been stated that chemotherapeutic agents cause unwanted results in male reproductive system due to the formation of DNA damage caused by oxidative stress and many antioxidants have protective effect against these effects. As a result, histopathological damage to the testicular tissue of MTX has been described. Dose and duration studies of Alpha Lipoic Acid (ALA) and other antioxidants should be performed against defined oxidative stress damage. The investigation of the possible protective effects of ALA is important in terms of both literature contribution and the protective effect of ALA in the use of MTX.

Keywords: Methotrexate; ALA; Cancer; Testis.

[1] Perez A, Woods A, Grattan CE (2009). Methotrexate: a useful steroid-sparing agent in recalcitrant chronic urticaria. *Br J Dermatol.* 2010 Jan; 162(1): 191-4.

[2] Bleyer WA, Poplack DG (1985). Prophylaxis and treatment of leukemia in the central nervous system and other sanctuaries [Review]. *Semin Oncol* 12:131-148.

[3] Padmanabhan S, Tripathi DN, Vikram A, Ramarao P, Jena G (2008). Cytotoxic and genotoxic effects of methotrexate in germ cells of male Swiss mice. *Mutation Research* 655: 59-6.

P-011

Characterisation of Produced Lipid from a Green Microalgae

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In recent years, an increase in the need for energy has increased the search for alternative energy sources to the point where the fossil fuel reserves, which meet most of the world's energy needs, have come to the exhaustion point. Renewable energy sources are important alternatives to fossil fuels and work towards the production and use of these fuels has gained momentum in Turkey and worldwide. The green microalgae *Haematococcus pluvialis* was evaluated as lipid producer microorganism. The use of several industrial waste as a carbon source will provide both an assessment of waste and a low cost of production contribution. Due to high production capacity and low prices, utilization of the crude glycerol as carbon source is one of the promising options for lowering the production cost. In this study the effect of different concentrations (1-10 mM) of crude glycerol, nitrogen (0-2.5 mM) and light intensity (0-4000 lux) on the growth of *H. pluvialis* CCAP34/12 was investigated. During incubation period total protein, carbohydrate and lipid concentrations were investigated by spectrophotometry. The produced lipid in optimum conditions was characterized with GC, FTIR and NMR. The produced lipid in optimum conditions contained stearic acid (32.07%), linoleic acid (14.33%), palmitic acid (11.96%), behenic acid (6.75%), elaidic acid (6.48%), α -linolenic acid (6.31%), myristic acid (4.89%). Spectra of NMR and FTIR demonstrated same functional group peaks (Fig. 1).

Due to the fatty acid content is related to fuel properties of lipid, it is important to identify the fatty acid composition. Additionally, other functional groups are also important for some properties such as viscosity, ignition point, sedimentation. According to the results, the produced lipid is suitable for biodiesel production. This study shows an alternative way to transform technical glycerol into a valuable product while showing that a waste is the appropriate carbon source for the production of a microalgae lipid with potential biodiesel potential.

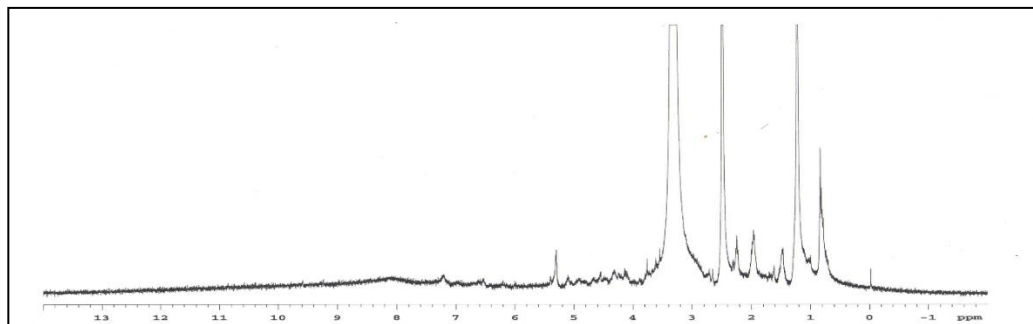


Figure 1. MNR spectrum of produced lipid from *H. pluvialis*.

Keywords: Lipid production; UV-visible spectroscopy; FTIR; NMR.

P-012

DFT Study of Band Structure of Poly(telluro[3,4b]tellurophene)

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Conjugated polymers have been subject to great interest since the doped polyacetylene as a conducting polymeric material was discovered [1]. Conjugated polymers have large chemical structure variations. As a result they have different electrical and optical properties. These type of polymers have wide range of applications based on their optical and electrical properties. For example, the conjugated polymer poly(thieno[3,4-b]furan) has been synthesized and theoretically analyzed [2]. In this study, the structure with the same skeleton but different heteroatom has been studied. Tellurium which is in the same group as with sulfur and oxygen is substituted to heteroatom positions. The obtained structure, poly(telluro[3,4b]tellurophene) (Fig.1) has been optimized using Gaussian 09 program package [3] within the periodic boundary conditions [4]. B3LYP hybrid functional [5] with the basis sets LANLDZ for Te and 6-31G(d,p) for the others has been employed for this purpose. There are four open positions to make bond with the neighbouring monomer. Some combinations of connection position are not appropriate to propagate chain. As a result, there are four possible connection positions for two monomers. The structure shown in Fig.1 is the structure formed via 4-6 positions. The structures with different connection positions have been studied. As a result of calculations, HOCO (Highest Occupied Crystal Orbital) and LUCO (Lowest Unoccupied Crystal Orbital) levels, band gap, band width, effective mass values have been obtained. It was concluded that the structure with 4-6 positions had the lowest band gap value. This result is compatible with the result of poly(thieno[3,4-b]furan). The values of other band structure quantities, band width and effective mass also shows that the structure with 4-6 connections is superior to others according to conducting properties.

Keywords: Conjugated polymers; HOCO; LUCO; Band gap; Effective mass.

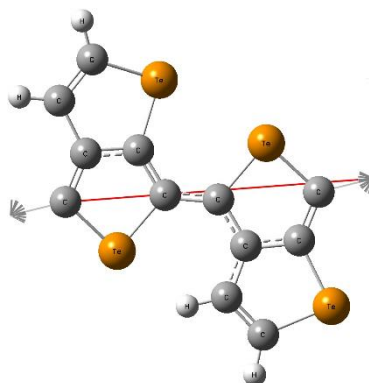


Figure 1. Structure of poly(telluro[3,4b]tellurophene).

- [1] C. K. Chiang et al., *Phys. Rev. Lett.*, 39, 1977, 1098-1101.
- [2] A. Kumar, J. G. Bokria, Z. Buyukmumcu, T. Dey, and G. A. Sotzing, *Macromolecules*, 41, 2008, 7098- 7108
- [3] Gaussian 09, Revision B.01, M. J. Frisch et al., Gaussian, Inc., Wallingford CT, 2010.
- [4] K. N. Kudin, G. E. Scuseria, *Phys. Rev. B*, 61, 2000, 16440-16453.
- [5] A. D. Becke, *Phys. Rev. A*, 38, 1988, 3098-3100.

P-13

The Use of Raman Spectroscopy in Forensic Sciences

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Forensic science can be broadly defined as the application of science to the law. Forensic scientists depend on reliable scientific instruments to provide accurate, detailed data that is admissible in court. As a result, choosing high quality instruments is paramount. Raman spectroscopy is useful for the investigation of molecular chemistry, and has the added benefits of being rapid, reliable and non-destructive. Raman data can be obtained from almost any surface, allowing minute traces of explosives or a firearm's discharge to be detected without attempting to lift samples from evidence. Raman spectroscopy is highly sensitive to minute chemical differences between inks. Images are generated in minutes, making this technique one of the fastest to characterize ink chemical structure.

It is used to analyze a plethora of forensic science samples including, but not limited to: drug pharmaceutical materials, geological materials, fibers, paints, inks and explosives, and can be extremely useful when facing any unknown component. In soil samples, Raman can be used not only to identify minerals but also to detect and confirm the identity of, for example, paint flakes and various biological materials. In this study, the use of raman spectroscopy in forensic sciences is discussed.

Keywords: Raman spectroscopy; Forensic science; Gun shot residue; Ink; Explosive; Soil.

[1] R. Saferstein, *Criminalistics: An Introduction to Forensic Science*, 2007, 213.

[2] Kammrath B, Koutrakosa A, Castillo J, Langley C, Huck-Jones D, *Morphologically-directed Raman Spectroscopy for Forensic Soil Analysis Forensic Science International*, 285, 2018, 25-33.

[3] Bueno J, Sikirzhytski V, Lednev I, *Raman Spectroscopic Analysis of Gunshot Residue Offering Great Potential for Caliber Differentiation, Trends in Analytical Chemistry*.

[4] Penido C, Pacheco M, Lednev I, Silveira L, *Identification of cocaine and other illegal drugs of abuse, Journal of Raman Scetroscopy*, 47, 2016, 28-38.

[5] Almaviva S, Palucci A, Botti S, Puiu A, Rufoloni A,, *Validation of a miniaturized spectrometer for trace detection of explosives by surfaceenhanced Raman spectroscopy*, 7, 2016, 1-8.

P-14

DFT Study of Polytellurophene as a H₂O Sensor

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Conducting polymers have been widely studied since the discovery of doped polyacetylene [1]. These polymers have wide application areas such as LEDs, gas sensors, batteries, electrochromic devices, photovoltaics, etc. As stated, they can also be used in the manufacture of gas sensors. It has been found that they are sensitive to gas molecules, organic molecules, pH, certain inorganic ions, etc. [2]. Molecular and electronic structure of polymers used as gas sensors can be studied by means of theoretical methods. Also, their sensing mechanism can be understood in this way. Bibi et al. have studied the sensitivity and selectivity of neutral and cationic pyrrole oligomers to NH₃, CO₂, and CO by DFT method. Polytellurophene which has the same skeleton as polypyrrole has been studied as an H₂O sensor in this study. The trimer of tellurophene has been optimized as a segment of the polymer. Then, the trimer of tellurophene with a H₂O molecule oriented to different positions has been optimized by DFT method to elucidate the sensing ability. B3LYP hybrid functional [4] with the basis sets LANLDZ for Te and 6-31G(d,p) for the others has been employed for the optimization and the calculation of additional properties. All the calculations have been carried out by Gaussian 09 program package [5]. The trimer of tellurophene with H₂O molecule directed to a certain position of the molecule is shown in Fig.1. Trimers with a H₂O molecule have been optimized with BSSE correction. After optimization of the trimers with H₂O oriented to the possible binding sites, binding energies, charge distributions, frontier molecular orbital energy levels have been calculated to see the effects upon adsorption of H₂O. According to the extent of the effect on these quantities, the best site for the sensing has been determined.

Keywords: Polytellurophene; Sensor; DFT; Binding energy; H₂O.

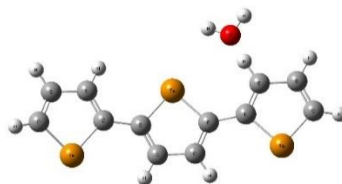


Figure 1. Trimer of tellurophene with H₂O molecule.

[1] C. K. Chiang et al., *Phys. Rev. Lett.*, 39, 1977, 1098-1101.

[2] U. Lange et al., *Anal. Chim. Act.*, 614(1), 2008, 1-26.

[3] S. Bibi et al., *J. Phys. Chem. C*, 119, 2015, 15994-16003.

[4] A. D. Becke, *Phys. Rev. A*, 38, 1988, 3098-3100.

[5] M.J. Frisch et al. Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford, 2010.

P-15

The Theoretical Investigation of Structural, Spectroscopic and Thermodynamic Properties of Palmitoleic Acid

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Palmitoleic acid (POA) is one of the most common omega-7 fatty acids, which is an unsaturated fatty acid in which the site of unsaturation is seventh carbon atom from the end of the carbon chain. POA is an important fatty acid for pharmaceutical applications and it is found in plants and marine sources. Macadamia nuts and buckthorn seed oil contain the cis isomer of POA and dairy products are rich sources of trans-palmitoleate [1].

To find the most stable conformers of POA, the potential energy surface (PES) scans were performed with the DFT/B3LYP/6-311++G(d,p) by rotation around C7-C8-C9-C10 and C9-C10-C11-C12 dihedral angles that the C-C bonds which are adjacent to C=C double bond located within unsaturated hydrocarbon chain and also by rotating the carboxylic group –COOH (O=C–O–H dihedral angle). The geometrical parameters and harmonic vibrational wavenumbers were calculated by the same method for the conformers. Quantum chemical descriptors (HOMO and LUMO energies, chemical hardness and softness, electronegativity, chemical potential) of the most stable conformers of POA were investigated theoretically in detail. Furthermore, some thermodynamic quantities such as entropy, heat capacity and Gibbs Free Energy of these molecules were calculated by DFT/B3LYP/6-311++G(d,p) method.

The optimized geometric parameters (bond lengths, bond angles and dihedral angles) and calculated vibrational frequencies of the most stable conformers of POA were compared with experimental results of X-ray crystal structure and experimental infrared frequencies of POA in the literature.

Keywords: Palmitoleic acid; Density Functional Theory (DFT); Conformers; Vibrational wavenumbers.

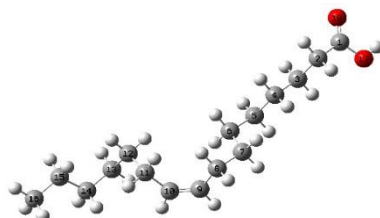


Figure 1. Chemical structure of Palmitoleic acid.

[1] Ernesto M. Hernandez, *Specialty Oils: Functional and Nutraceutical Properties. Functional dietary lipids*, 2016, Sawston, UK: Woodhead Publishing, pp. 69-100.

P-16

Spectroscopic and Thermal Study of 3D-Metal Complexes with Pyrazolecarboxylic Acid

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In this work, the thermal and spectroscopic properties of 3d-metal (Co, Cu, Zn, Mn, Ni) and sodium salts with pyrazole-3-carboxylic acid and pyrazole-4-carboxylic acid were studied. The IR and Raman spectra were registered and analyzed in the range of 400–4000 cm⁻¹. The thermogravimetric study of synthesized compounds was done. The degree of hydration and the products of thermal decomposition were estimated. The complexes of pyrazole-3-carboxylic acid acid have the general formula: M(C₄H₃N₂O₂)₂·nH₂O where M = Mn, Fe, Co, Ni, Cu, Zn, n = 2 for zinc complex, n=3 for copper, n=2.5 for cobalt, manganese and nickel complex was anhydrous. The complexes of pyrazole-4-carboxylic acid have the general formula: M(C₄H₃N₂O₂)₂·nH₂O where M = Mn, Fe, Co, Ni, Cu, Zn, n = 2 for copper complex, n=4 for nickel, n=4.5 for cobalt complex, manganese and zinc complex was anhydrous. Moreover, it was done the comparison between the effect of 3d-transition metal cations and sodium cation on the degree of perturbation or stabilization of the electronic system of pyrazole molecule depending on the position of carboxylic group in the ring. The spectroscopic studies showed that the 3d-transition metals stabilize the electronic system of studied acids.

Keywords: Pyrazole-3-carboxylic acid; Pyrazole-4-carboxylic acid; Pyrazole; Thermal study.

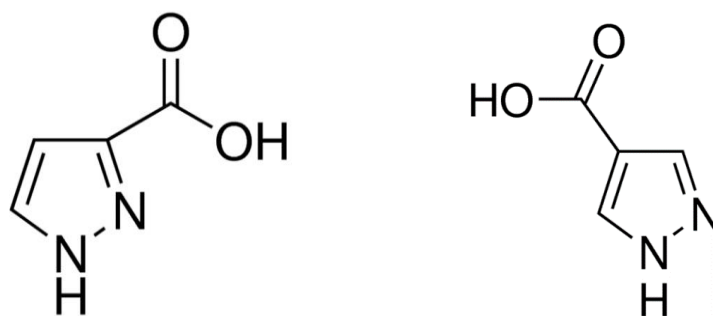


Figure 1. Structural formula of pyrazole-3-carboxylic acid and pyrazole-4-carboxylic acid.

P-17

Spectroscopic Study on Alkali Metal Salts of Rosmarinic Acid

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The molecular structure of alkali metal rosmarinates was studied in comparison to rosmarinic acid using FT-IR, FT-Raman, ¹H and ¹³C NMR spectroscopy as well as density functional theory (DFT) calculations. The B3LYP/6-311+G(d,p) method was used to calculate the optimized structures of studied compounds, atomic charges, dipole moments, energies, some general reactivity descriptors as well as the wavenumbers and intensities of the bands from the vibrational and NMR spectra. The relationship between the spectroscopic data and theoretical parameters of studied compounds was analyzed. The antioxidant activity using DPPH and FRAP tests and photochemical properties were determined. Good correlation was found between the HOMO and LUMO orbital energies and the reducing power expressed as FRAP ($R^2=0,936$). The linear correlation between reaction rates and energy gap between HOMO and LUMO levels was observed ($R^2=0,992$). Energy of HOMO/LUMO orbitals and other reactivity descriptors show that the electron affinity, electronegativity and electrophilicity index decrease in series acid > K > Li > Na salt. It indicates that the acid has higher electrophilic power (higher electron transfer ability) than alkali metal rosmarinates. While it was found that alkali metal rosmarinates have better antioxidant properties than rosmarinic acid and the highest antioxidant activity has been found for the sodium salt.

Keywords: Rosmarinic acid; Alkali metals; Antioxidant properties; Photochemical properties.

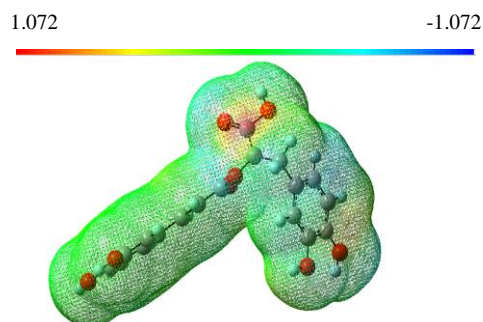


Figure 1. The distribution of electron density in molecules of rosmarinic acid.

Acknowledgements

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P-18

Pro-, Antioxidant, Cytotoxic (toward MCF-7 and MDA-MB-21 Cell Lines), Lipophilic and Antimicrobial Activity of Hydroxybenzoic Acids

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The plant hydroxybenzoic acids possess different physico-chemical and biological properties depending on the number and position of the hydroxyl substituents in the ring [1, 2]. In this study the relationship between the structure and the biological (antioxidant, cytotoxic, lipophilic and antimicrobial) activity of dihydroxy- and trihydroxybenzoic acids was studied. Different spectroscopic assays were applied in order to establish the biological properties of compounds. The antioxidant activity was studied using a stable free radical α , α -diphenyl- β -picrylhydrazyl (DPPH), ferric and cupric reducing antioxidant potential (FRAP and CUPRAC) assays. The pro-oxidant effect of compounds on trolox oxidation was measured. The neutral red (3-amino-7-dimethylamino-2-methyl-phenazine hydrochloride) uptake assay for the estimation of cell viability/cytotoxicity was applied. The chromatographic lipophilicity parameters obtained under different chromatographic condition were obtained. The MIC (minimal inhibitory concentration) against different bacteria and yeast strains (*Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Bacillus subtilis*, *Salmonella enteritidis* and *Candida albicans*) was obtained. The statistical analysis of the obtained parameters was done in order to study the structure-activity relationship.

Keywords: Hydroxybenzoic acids; Antioxidant; Antimicrobial; Cytotoxic; Lipophilic.

Acknowledgements

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[1] M. Kalinowska, L. Mazur, E. Regulska, A. Korczak, G. Świdorski, W. Lewandowski, *Journal of Coordination Chemistry*, 69, 2016, 2415-2421.

[2] M. Kalinowska, L. Mazur, A. Jabłońska-Trypuć, W. Lewandowski, *Journal of Saudi Chemical Society*, 22, 2018, 742-756.

P-19

Comparison of Spectroscopic and Thermal Properties of 3D-Metal Complexes with Nicotinic and Quinolinic Acid

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Ligands, which are pyridine derivatives, including pyridinecarboxylic and pyridinedicarboxylic acids are of great biological importance. These compounds, due to the presence of nitrogen in the pyridine ring, can form stable chelates with different types of coordination, joining complexes with metals not only through the carboxyl group but also through the nitrogen atom. A number of them form complexes with coordination (N, O-metal). As a result, pyridinecarboxylic and pyridinedicarboxylic acids are potential natural chelators.

In this work, the spectroscopic (IR, Raman, UV-Vis) and thermal properties of 3d metal complexes with nicotinic and quinolinic acid were studied in order to determine the effect of 3d metals [i.e., Mn(II), Co(II), Ni(II), Cu(II), Zn(II)] on the electronic structure and physicochemical properties of the ligand. The spectroscopic studies showed that the 3d-transition metals stabilize the electronic system of studied acids. The complexes of nicotinic acid have the general formula: $M(C_6H_4NO_2)_2 \cdot 2H_2O$ where $M = Mn, Fe, Co, Ni, Cu, Zn$, $n = 2$ for manganese complex, $n=4$ for cobalt, zinc and nickel complex, copper complex was anhydrous. The complexes of quinolinic acid have the general formula: $MC_7H_3NO_4 \cdot nH_2O$ where $M = Mn, Fe, Co, Ni, Cu, Zn$, $n = 2$ for zinc complex, $n=3$ for cobalt and nickel complex, $n=4$ for manganese complex copper complex was anhydrous.

Keywords: Nicotinic acid; Quinolinic acid; Metal complexes; Pyridinecarboxylic acid.

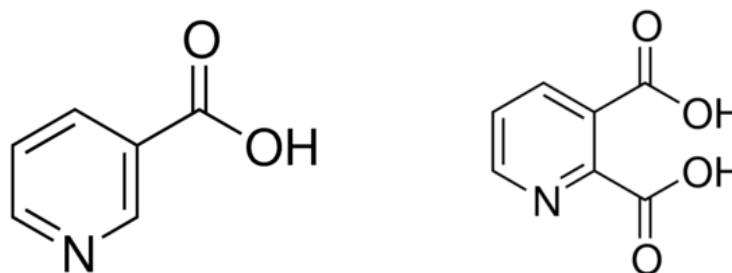


Figure 1. Structural formula of nicotinic and quinolinic acid.

P-20

The Effects of the Metallic Synergy in the Barbiturate and Borat Complexes on Thermal Degradation of PVC

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Some metal complexes used as thermal stabilisers are applied in the PVC blend for thermal stabilization. PVC is unstable molecule. During the thermal degradation of PVC, H⁺ and Cl⁻ ions are released from the molecular structure. In this time, the concentrations of the HCl gas rate will be increased. This situation occurs unsuitable effects on the human health. The thermal degradation of the PVC are got resist or delayed via thermal stabilizer materials in the PVC blend. Our previously study, the thermal stabiliser effects of the borate and barbiturate complexes were published [1]. This study is extended with the metallic synergy effects of M₁(III)/M₂(II) atoms [where M₁: Cr(III), Al(III) or M₂(II): Mn(II), Co(II) or Ni(II)]. The molecular structures of the synthesized complexes as thermal stabiliser materials are investigated by elemental analysis, vibrational (FT-IR and Raman) spectroscopy, X-ray diffraction (XRD) and X-ray fluorescence (XRF) methods, and thermal analyses (TG, DTA and DTG) techniques. The thermal resistant capacities of the complexes are obtained with thermostatic analysis, which is described in ISO 182-2 standards. Then, obtained thermostatic analysis results are compared with thermostatic analysis results of the conventional PVC blend. These results are shown that the synthesized complexes are demonstrated good thermal stabiliser behaviors.

Keywords: Thermal degradation of PVC; Thermal stabilizer; Metal complexes; ISO 182-2; Vibrational spectroscopy; X-ray diffraction.

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[1] İlkan Kavlak, Güneş Süheyla Kürkçüoğlu, Onur Şahin, *Journal of Molecular Structure*, 1184, 2019, 418-426.

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The Investigation of Thermal Stabilization Properties of The M(II) Barbiturate Complexes in the PVC Mold

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In our study, the thermal stabilization properties of the Cu(II), Cd(II) and Sn(II) complexes were investigated with thermostatic analysis method which is described in ISO 182-2 standard [1]. The previous study is extended with new generation thermal stabilisers which is made of Mn(II), Co(II) or Ni(II) barbiturate complexes. During the thermal degradation of PVC, H⁺ and Cl⁻ ions are released from the PVC molecule. Hence, the concentrations of the HCl gas rate will be increased. This situation occurs unsuitable effects on the PVC quality and human health. The thermal degradation of the PVC are got resist or delayed via thermal stabilizer materials in the PVC blend. The complexes obtained as thermal stabilizing materials are examined by elemental analysis, vibrational (FT-IR and Raman) spectroscopy, X-ray diffraction (XRD) and X-ray fluorescence (XRF) methods, thermal analyses (TG, DTA and DTG) techniques. The thermal stability properties of the complexes are determined with thermostatic analysis, which is described in ISO 182-2 standards. Additionally, the thermostatic analysis results are compared with thermostatic analysis results of the conventional PVC blend. As a result, the synthesized complexes have good thermal capability during the PVC degradation.

Keywords: Thermal degradation of PVC; Thermal stabilisers; Metal complexes; ISO 182-2; Vibrational spectroscopy; X-ray diffraction.

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[1] İlkan Kavlak, Güneş Süheyla Kürkçüoğlu, Onur Şahin, *Journal of Molecular Structure*, 1184, 2019, 418-426.

P-22

Strong Shock Indication in Kemer Meteorite: Implications from Infrared Spectroscopy

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Kemer meteorite (KM) that fell in Muğla, Turkey in 2008 has been classified as an ordinary chondrite and falls into L4 group. It was reported as matrix poor chondrule rich meteorite and consists of diopside, chromite and feldspar. Olivine Fa was reported to be between 24–25% [1]. We successfully determined strongly shocked pyroxene signals from the observed bands at 836, 879, 944, 970 and 1000 cm^{-1} in IR spectrum of KM and found that KM meteorite has mean Fo composition of 75% [2, 3]. Fo composition were also confirmed from the peaks at 1000, 970, 880, 836, 589, 515, 494 cm^{-1} . Olivine shock profile was also investigated by the peak intensity at 970 cm^{-1} and peak shift between 862–875 cm^{-1} (879 cm^{-1} in KM). Peak shift of about 17 cm^{-1} indicates that KM has also strongly shocked olivine. However, in general, lower IR absorbance values lower than 0.3 is another indication of the existence of shocked minerals.

Keywords: Kemer meteorite; IR spectroscopy; Pyroxene; Olivine.

[1] The Meteoritical Bulletin. 2012. 99:E2.

[2] Kereszturi A., Gyöllai I., Kereszty Zs., Kiss K., Szabó, Szalai Z., Ringer M., and Veres M. 2017. Analyzing Raman – Infrared spectral correction in the recently found meteorite Csátalja. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 173:637-646.

[3] Lane M. D., Glotch T. D., Dyar M. D., Pieters C. M., Klima R., Hiroi T., Bishop J. L., and Sunshine J. 2011. Midinfrared spectroscopy of synthetic olivines: Thermal emission, specular and diffuse reflectance, and attenuated total reflectance studies of forsterite to fayalite. *Journal of Geophysical Research* 116:E08010.

P-23

Donor-acceptor π -conjugated Naphtalene Bis–benzimidazole: A DFT, Infrared and Raman Spectroscopic Study on a Heterojunction Solar Cell

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This study represents the first time detailed vibrational analysis of naphtalene bis–benzimidazole (NBBI) by Attenuated Total Reflectance (ATR) Fourier Transform Infrared (FTIR) and Raman spectroscopy supported by quantum chemical studies. The motivation of this investigation is that NBBI is an n-type organic thin film phototransistor which can be used as organic semiconductors which of great interest and there is a strong need of low–cost, high–efficiency heterojunction solar cell (HSCs) [1,2]. In order to investigate vibrational features of NBBI, FTIR and Raman spectra were recorded between 4000–650 cm^{-1} and 4000–50 cm^{-1} at room temperature, respectively. Optimized molecular structure and vibrational wavenumbers of the compound in its ground state have been calculated by using Density Functional Theory (DFT) using B3LYP functional with 6-311++G(d,p) basis set by Gaussian 09 software [3]. Vibrational wavenumbers were seen to be in good agreement with the experimental data. Furthermore, detailed assignments of each vibrational modes were interpreted in terms of potential energy distributions in detail by Veda 4 software [4]. Besides, due to their key role in understanding light harvesting effects of HSCs, there is also an urgent need to focus on intramolecular bond distances according to Natural Bond Order (NBO) charges on donors and acceptors and we also calculated NBO charges. Effect of the nature and length of π -linker was also discussed in this study. We also reported Highest Occupied Molecular Orbitals (HOMO) and Lowest Unoccupied Molecular Orbitals (LUMO) since these orbitals play a key role in designing such light harvesting systems.

Keywords: Naphtalene bis–benzimidazole; ATR–FTIR; Raman; Heterojunction solar cells; Organic solar cells.

[1] B. Oregan, M. Grätzel, Nature, 353 (1991) 737-740.

[2] J.Q. Li, L. Wang, Q. Zhang, W.P. Wu, C.Z. He, J.L. Zhang, Org Electron, 22 (2015) 108-116.

[3] G.W.T. M. J. Frisch et al., Gaussian 09 (Gaussian, Inc., Wallingford CT, 2009), (2009).

[4] M.H. Jamróz, Vibrational Energy Distribution Analysis VEDA 4, Warsaw, 2004, (2004).

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Vibrational Spectroscopic and DFT Investigation on Electron Acceptor Perylene Bisbenzimidazole

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In this study, the experimental and theoretical results on the molecular structure of perylene bisbenzimidazole (PBBi) by Attenuated Total Reflectance (ATR) Fourier Transform Infrared (FTIR) and Raman spectroscopy are presented for the first time. Organic dye films are extensively used in electronic and optoelectronic devices like light-emitting diodes, heterojunction solar cells and transistors [1–4]. Solid state organic solar cells are interesting due to the reason developing inexpensive, efficient and renewable energy sources [5,6]. We calculated vibrational wavenumbers of PBBi and optimized its molecular structure in its ground state by using Density Functional Theory (DFT) with B3LYP functional with 6-311++G(d,p) basis set by Gaussian 09 software [7]. FTIR and Raman spectra were recorded between 4000–650 cm^{-1} and 4000–50 cm^{-1} at room temperature, respectively. The first-time detailed assignments of each vibrational modes were interpreted in terms of potential energy distributions by Veda 4 software [8].

Keywords: Perylene bisbenzimidazole; ATR–FTIR; Raman, Heterojunction solar cells; Organic solar cells.

[1] C.W. Tang, Appl. Phys. Lett. 48, 183 (1986).

[2] C.J. Brabec, N.S. Sariciftci, J.C. Hummelen, Adv. Funct. Mater. 11, 15 (2001).

[3] M.T. Bernius, M. Inbasekaran, J. O'Briben, W. Wu, Adv. Mater. 12, 1737 (2000).

[4] Y.Z. Wang, R.G. Sun, D.K. Wang, T.M. Swager, A. Epstein, Appl. Phys. Lett. 74, 2593 (1999).

[5] J. Rostalski, D. Meissner, Sol. Energ. Mat. Sol. C. 61, 87 (2000).

[6] M. Westphalen, U. Kreibitz, J. Rostalski, H. Lüth, D. Meissner, Sol. Energ. Mat. Sol. C. 61, 97 (2000).

[7] G.W.T. M. J. Frisch, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09 (Gaussian, Inc., Wallingford CT, 2009), (2009).

[8] M.H. Jamróz, Vibrational Energy Distribution Analysis VEDA 4, Warsaw, 2004, (2004).

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Characterization of Proteins by Vibrational Spectroscopy and Self-Organizing Maps

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Antibodies are one of the top biopharmaceuticals market type due to their applications in oncology therapy. However, they can undergo changes at different structural levels that can result in loss of their activity [1]. Although mass spectrometry is a powerful technique for primary structure determination, it fails to give information at higher order levels. In this project we explored the possibilities of vibrational spectroscopic techniques as a tool kit to help ensure the integrity and batch to batch reproducibility in antibody manufacture.

Infrared (IR) and Raman spectra are well known to contain bands (Amide I, II and III) with shapes that correlate to secondary structure (SS) [2][3][4]. Unlike Circular Dichroism (CD) (the most well-established technique for secondary structure analysis [5]), IR and Raman spectroscopy allow much wider ranges of optical density which makes the analysis of complex pharmaceutical samples more feasible. However, the data processing and extraction of this information are ambiguous and, in many cases, limited by spectral noise and water absorption in IR and fluorescence in Raman. A neural network algorithm that we called self-organizing maps (SOMspec) was implemented for the prediction of SS by fitting the Amide I with a reference set of proteins of known SS. Data sets of proteins were collected in both solid and aqueous state by Raman, IR and Raman Optical Activity. The proteins used for the experiments were commercial ones with the highest possible SS coverage. The results presented in figure 1 correspond to those of solid state by Raman. Although in general pretty accurate, for some of the proteins the predictions were far from expected meaning the reference sets might not be large enough or the shape of the bands are not always univocal to SS as thought. Complementary analysis of the Amides II and III are to be performed in the near future.

Keywords: Proteins; Secondary structure; Raman; Infrared; Neural network.

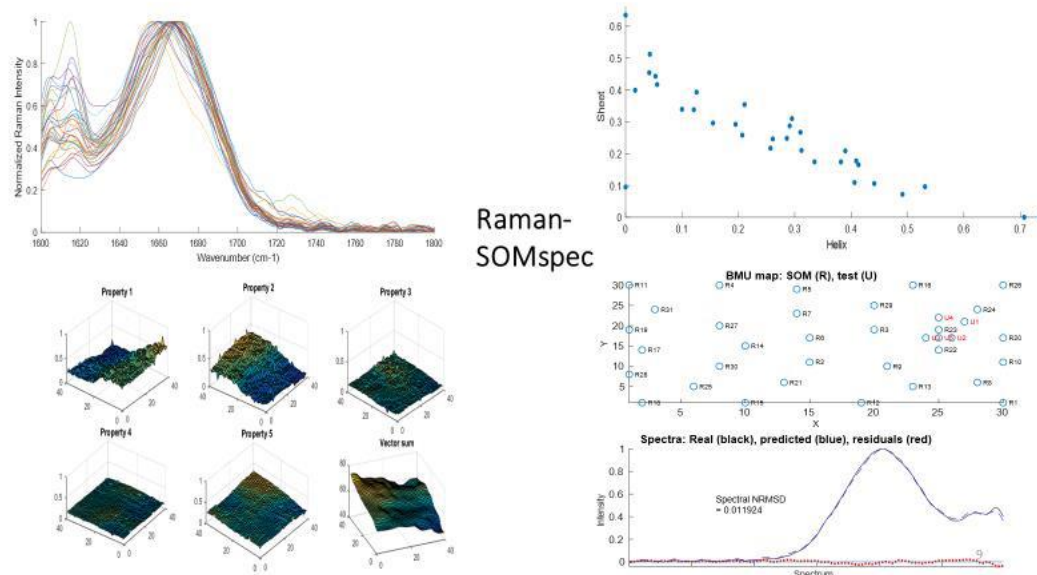
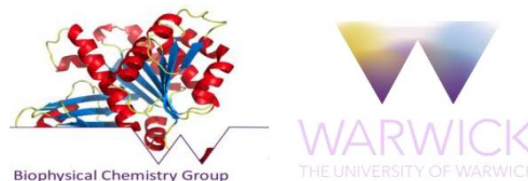


Figure 1. Raman reference set (upper-left), coverage of helical and beta strand structures (upper-right), SOM map and fitted protein (lower-right) and distribution of properties on the map (lower-left).

Acknowledgements



- [1] S. Ausar, Hasija, Li, and Rahman, "Forced degradation studies: an essential tool for the formulation development of vaccines," *Vaccine Dev. Ther.*, 2013, pp. 11.
- [2] J. Kong and S. Yu, "Fourier Transform Infrared Spectroscopic Analysis of Protein Secondary Structures Protein FTIR Data Analysis and Band Assign- ment," vol. 39, no. 8, 2007, pp. 549–559.
- [3] A. Barth, "Infrared spectroscopy of proteins," vol. 1767, 2007, pp. 1073–1101.
- [4] A. Rygula, K. Majzner, K. M. Marzec, A. Kaczor, and M. Pilarczyk, "Raman spectroscopy of proteins : a review," no. July, 2013, pp. 1061–1076.
- [5] S. M. Kelly, T. J. Jess, and N. C. Price, "How to study proteins by circular dichroism," vol. 1751, 2005, pp. 119–139.

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